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COORDINATORE: PROF. SALVATORE CAPOZZIELLO

Hamilton-Jacobi Methods in Fields, Particles and Information Geometry

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Tutore:

Prof. Giuseppe Marmo

Dottorando:

Fabio Di Cosmo

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Introduction

The central point around which this thesis has been developed is the investigation of geometrical structures which are present in some theories of increasing interest in physics. In particular attention has been focused on information theory and quantum mechanics, where the systematic use of specific coordinate systems makes extremely difficult a proper geometrical interpretation of their contents.

A guiding principle in this investigation has been the search for analogies with situations where the role of tensorial structures is better understood, first of all the realm of Lagrangian and Hamiltonian mechanics. Interestingly a unifying feature of all this investigation has been Hamilton-Jacobi theory and particularly its relationship with the definition of generating functions of canonical transformations. Indeed complete solutions of Hamilton-Jacobi equation generate symplectic diffeomorphisms which permit to map tangent bundle $T\mathcal{M}$ or cotangent bundle $T^*\mathcal{M}$ of a carrier space \mathcal{M} onto two copies $\mathcal{M} \times \mathcal{M}$ of the same carrier space.

Let $T^*\mathcal{M}$ be the cotangent bundle over a n -dimensional configuration space \mathcal{M} and let (q^j, p_j) define a local coordinate system of $T^*\mathcal{M}$. In these coordinates the canonical symplectic structure ω_0 on $T^*\mathcal{M}$ is written as follows:

$$\omega_0 = \sum_{k=1}^n dp_k \wedge dq^k, \quad (1)$$

whereas an associated Liouville potential one form is

$$\theta_0 = \sum_{k=1}^n p_k dq^k. \quad (2)$$

A symplectic diffeomorphism on $T^*\mathcal{M}$ from (q^k, p_k) to (Q^k, P_k) is assigned once a generating function $S(q, Q; t)$ satisfying the condition

$$\det \left| \frac{\partial^2 S}{\partial q^j \partial Q^k} \right| \neq 0, \quad (3)$$

is given. In particular such a diffeomorphism is obtained according to the following formulae:

$$p_k = \frac{\partial S}{\partial q^k} \quad (4)$$

$$P_k = -\frac{\partial S}{\partial Q^k}. \quad (5)$$

If $H(q, p, t)$ is a Hamiltonian function on $T^*\mathcal{M}$ the transformed Hamiltonian is $K = H + \frac{\partial S}{\partial t}$. If K can be chosen to vanish the system can be reduced to equilibrium and $S(q, Q, t)$ is a complete solution of the following Hamilton-Jacobi equation:

$$\frac{\partial S}{\partial t} + H\left(q, \frac{\partial S}{\partial q}, t\right) = 0, \quad (6)$$

which generally is a non-linear first-order PDE.

If the variables Q^k define the configuration of the system at a fixed time T and q^k at a different instant t , a complete solution of (6) can be written as follows

$$S(q, Q, t) = \int_t^T \mathcal{L} dt, \quad (7)$$

where the integral is evaluated along a solution of equations of the motion which passes through the point $Q^k(T)$ and $q^k(t)$ and $\mathcal{L} = \sum_k \dot{q}^k p_k - H$ is the lagrangian function associated with the dynamical system. Such an integral is called Hamilton principal function and it will play an important role in information geometry, as it will be shown in the third chapter.

It is possible to look at the theory of generating functions from a more “geometrical” point of view.¹ Indeed let us consider the product manifold $T^*\mathcal{M} \times T^*\mathcal{M}$ and let π_1 and π_2 be the associated projections onto the first and the second factor of the product.

Since $T^*\mathcal{M}$ is a symplectic manifold with respect to the canonical two form ω_0 , the two form $\omega = \pi_1^*(\omega_0) - \pi_2^*(\omega_0)$ on $T^*\mathcal{M} \times T^*\mathcal{M}$ defines a symplectic structure on the product manifold. An associated Liouville one-form is $\theta = \pi_1^*(\theta_0) - \pi_2^*(\theta_0)$.

The graph $\Sigma \equiv ((q, p), \phi(q, p))$ of a symplectic diffeomorphism $\phi : T^*\mathcal{M} \rightarrow T^*\mathcal{M}$ determines a submanifold of the product manifold $T^*\mathcal{M} \times T^*\mathcal{M}$ which is a Lagrangian submanifold with respect to the symplectic two form ω . Therefore the following chain of equalities is valid:

$$0 = \omega|_{\Sigma} = d\theta|_{\Sigma}, \quad (8)$$

¹This geometrical aspect has been used in order to define Hamilton-Jacobi theory also at the level of Lagrangian mechanics on the tangent bundle $T\mathcal{M}$ (for more details see [1])

and consequently there exists locally a function S_ϕ on Σ such that

$$\theta|_\Sigma = dS_\phi. \quad (9)$$

This function is the generating function of the symplectic diffeomorphism ϕ and the equation (9) can be rewritten in the more familiar form²

$$\sum_k (p_k dq^k) - \sum_k (P_k dQ^k) = dS_\phi(q, Q). \quad (10)$$

Hamilton-Jacobi theory, however, is not only a useful tool in Hamiltonian description of particle mechanics. During the 60's Peter Bergmann [3, 4], and Arthur Komar [5, 6] proposed a Hamilton-Jacobi formulation of General Relativity based on the Hamiltonian formulation introduced same years before by Dirac [7, 8]. This formulation was characterized by the presence of four first-class constraints (for more details on Dirac theory of constraints see [9]), let us call them C^a , associated with the reparametrization freedom of Einstein theory. Bergmann and Komar, therefore, considered these constraints as Hamiltonians and used them in order to write four Hamilton-Jacobi equations for a functional $S[g]$ of the metric tensor, g . Furthermore this functional was interpreted as the generating functional of a canonical transformation mapping the initial phase space of the theory to the constrained one.

Mappings like (10) will be widely adoperated in this thesis in order to move from a description in terms of configurations and “velocities” or “momenta” to a description in terms of pairs of configurations. This is extremely useful in order to avoid the use of “velocities” in theories where “velocities” or “momenta” do not possess a direct physical measurable interpretation, like statistics and information theory or classical and quantum field theory.

Another central topic where the role of this kind of transformations will be investigated is covariant relativistic description of field theories. The main feature of this “picture” is the avoidance of a splitting of space-time into space and time. Many poposals have been advanced in order to define brackets depending on the values of the dynamical fields at different points of the spacetime, instead of equal-time (such a kind of bracket is fundamental in order to understand how to formulate Quantum Mechanics in a relativistic setting). Therefore it is natural to ask whether canonical transformations mapping a cotangent bundle $T^*\mathcal{M}$ into two copies of the configuration space $\mathcal{M} \times \mathcal{M}$ could play a role in such a kind of covariant description.

Apart from the fact that general relativity has forced physicists to translate physical ideas in the language of differential geometry, understanding the

²This formula can be generalzed also to include one-parameter group of diffeomorphism in the so called extended formalism (see for instance [2]).

geometrical content in the description of a physical system is extremely useful in order to build generalizations in a proper way. Furthermore a deeper comprehension of the mathematical description of a system is necessary in order to find analogies with other theories: these analogies are fundamental in any scientific discipline since they promote an exchange of ideas and consequently an increase of knowledge. Therefore in this thesis it will be presented an investigation of some aspects of some physical systems from a more geometrical perspective: Quantum Mechanics, covariant description of particles and fields and Information Geometry share, in fact, some common features related with the theory of canonical transformation.

Let us now take a closer look at the structure of the thesis. It is divided into three chapters.

In the first chapter we will start with some considerations on quantum-to-classical transitions. After recalling the WKB method, we will illustrate how classical-like dynamics can be obtained by reducing the initial Hilbert space associated with a quantum system to a manifold of selected states. Then the discussion will move towards the possibility of introducing a variational principle in order to define dynamical evolution of Quantum Systems. In particular the proposals advanced by Dirac and Schwinger will be properly analyzed. Both of them, in fact, focused on the relationship between variational principles and the theory of canonical transformation: in particular they considered propagators as the analogue of generating functions. We will mainly focus on the approach proposed by Schwinger providing also some interesting examples. Furthermore in the last part of the chapter it will be shown directly by means of an example how Schwinger extended his variational principle also to field theories [10] and how it is possible to use this formulation to generalize Hamilton-Jacobi theory to a relativistic setting without breaking covariance.

Covariant description of relativistic physical systems will be the topic of the second chapter. In particular the definition of Peierls bracket [11] both for particle and fields dynamics will be presented from a more geometrical point of view. Peierls bracket is a bracket which involves the values of dynamical fields at different points of the spacetime and it was widely used by de Witt [12] in its covariant description of gravitational field. In this second chapter we will focus mainly on the geometrical interpretation of Peierls' prescription and this will allow us to generalize Peierls' idea in order to define a Jacobi structure on the space of geodesics. According to Kirillov theorem [13] this kind of geometrical structure is the most general antisymmetric bilinear operator which satisfy a locality requirement.

Third chapter will be devoted to Information Geometry. Information

geometry was born as a geometrical study of the problem of statistical inference. After a short review of the main concepts and definitions of Information Geometry, it will be explained how Hamilton principal function (7) can be used in order to introduce a “canonical” potential function for a given statistical model. Potential functions are two-points functions which generalize the concept of divergence functions. They allow to recover all tensors which characterize a statistical model (Ξ, g, T) : Ξ is a manifold the points of which are probability distributions, g is a metric tensor and T is a symmetric tensor of degree three, called skewness tensor. Since there is not a unique potential function which determines a given statistical model, this chapter will advance a proposal in order to select a “canonical” one.

Chapter 1

Hamilton-Jacobi methods in Quantum Dynamics

The subject of this chapter is the analysis of the role of Hamilton-Jacobi theory and contact transformations in the development of Quantum descriptions. We will begin with a summary of the WKB method for solving Schrödinger equation: it can be transformed into a pair of coupled partial differential equations involving the amplitude $A(x,t)$ and the phase $S(x,t)$ of the wave function. In the short wave-length limit when $\hbar \rightarrow 0$ these two equations decouple and one reduces to the Hamilton-Jacobi equation of a particular classical Hamiltonian system. A different way of looking at classical-like dynamics of a Quantum system proposed in a recent paper [14] employs the quantizer-dequantizer formalism and the definition of suitable systems of coherent states. Both these procedures, indeed, allow to define submanifolds of states of the Hilbert space associated with a quantum systems. A Quantum dynamics which suitably reduces to these sets of states will be called classical-like and conditions under which the induced motion on the manifold of states is completely integrable are provided.

A different perspective is adopted in the second part of the chapter. Indeed during the development of Quantum Theory eminent scientists investigated the possibility of defining contact transformations in a quantum framework. In particular in this section we will present the ideas exposed by Dirac and Schwinger about quantum transformation functions, which are kernels of integral operators that allow to change the representation of the Hilbert space associated with a given Quantum System. Both of them found an analogy between these transformation functions and variational formulations.

In particular we will dedicate more time to Schwinger's formulation of Quantum dynamics, which is based on a variational principle, and to its deep relations with Hamilton-Jacobi theory. Firstly we will describe this principle

for the case of non relativistic Quantum Mechanics of particles, revisiting the usual examples of free particle and harmonic oscillator. Then we will introduce the extension of these results to the theory of Quantized fields made by Schwinger during the 50's. This analysis allows to define a generalization of Hamilton-Jacobi equation to relativistic field theories. The section closes with the example of the free Lagrangian of the Klein-Gordon field.

1.1 Dynamical Aspect in the Quantizer-Dequantizer Formalism

In this first section, following the paper [14], we will expose how it is possible to define classical-like dynamics for a Quantum systems according to a reduction procedure. Reduction will require the definition of a generalized Weyl system or of a set of generalized coherent states, which will provide the immersion of a manifold M into the Hilbert space \mathcal{H} associated with a Quantum system: this will introduce a non-linear element in a linear theory.

Indeed, the mathematics of Quantum Mechanics entails linear structures in the Hilbert space \mathcal{H} of the system, in the dynamical evolution given by Schrödinger equation, and in the set of linear operators on \mathcal{H} . On the other hand, the degrees of freedom of a classical physical system are generally modelled on non-linear manifolds, and the dynamical evolution needs not allow for any superposition rule.

Consequently, to better understand the quantum-to-classical transition it is conceivable that the introduction of nonlinear changes of coordinates in Quantum Mechanics may make the analysis more clear. An example of such a classical limit procedure is given by the so-called WKB short-wave limit of Schrödinger equation which will be now briefly recalled.

Let $\psi(x, t)$ be a wavefunction in the Hilbert space $\mathcal{H} = \mathcal{L}^2(\mathbb{R}^n, d\mu)$, where $d\mu$ is the Lebesgue measure on \mathbb{R}^n , and consider the Schrödinger equation:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi + V(x)\psi \quad (1.1)$$

Using a polar representation $\psi(x, t) = A(x, t) e^{-\frac{i}{\hbar}W(x,t)}$, where the functions A and W are real, and A is strictly positive, the Schrödinger equation (1.1) becomes a system of two coupled partial differential equations:

$$\frac{\partial W}{\partial t} = \frac{1}{2m} |\nabla W|^2 + V(x) - \frac{\hbar^2}{2m} \frac{\Delta A}{A}, \quad (1.2)$$

$$\frac{\partial A}{\partial t} = \frac{1}{2m} (2\nabla A \cdot \nabla W + A\Delta W). \quad (1.3)$$

We would like to stress that this is a nonlinear change of coordinates in a realization of the Hilbert space which makes the superposition rule, appropriate for the description of interference phenomena, quite nontrivial.

Now, one may perform what is known as the classical limit of the Schrödinger equation, which amounts to take the limit in which \hbar goes to 0. It is clear that the only term which is affected by this limiting procedure is the third one in the right hand side of equation (1.2). Clearly, when $\frac{\Delta A}{A}$ is bounded, if \hbar goes to 0, so does $\frac{\hbar^2}{2m} \frac{\Delta A}{A}$, and thus one can neglect the third term in equation (1.2). The result is that the system of equations is no longer coupled, and Eq. (1.2) reduces to the Hamilton-Jacobi equation:

$$\frac{\partial W}{\partial t} = \frac{1}{2m} |\nabla W|^2 + V(x), \quad (1.4)$$

associated with the Hamiltonian function $H = \frac{1}{2m} p^2 + V(x)$ plus an equation that will be recognized as a continuity equation.

Remark 1 *In the case in which $A = 0$ at some isolated points, that is, the wavefunction ψ has nodes, the third term of equation (1.2) could present divergences, and thus one should previously check that $\frac{\Delta A}{A}$ presents no divergences on the nodes, and then proceed as illustrated above. If $\frac{\Delta A}{A}$ actually presents divergences, than the procedure outlined can not be applied to the quantum state described by the wavefunction ψ .*

When one is dealing with a time-independent Hamiltonian, it is possible to make the following ansatz for the solution of equation (1.4):

$$W(x, q, t) = S(x, q) + Et \quad (1.5)$$

where E is a constant and q are parameters that will be identified with the final coordinates of the system. Then Eq. (1.4) reduces to the time-independent Hamilton-Jacobi equation

$$\frac{1}{2m} |\nabla S|^2 + V(x) = E. \quad (1.6)$$

Once a complete solution $S(x, q)$ of the Hamilton-Jacobi equation is determined, it can be shown that

$$A^2 = \left| \det \left(\frac{\partial^2 S}{\partial x^j \partial q^k} \right) \right|,$$

is a solution of Eq. (1.3). Let us recall that a complete solution of the Hamilton-Jacobi equation is a function $S(x, q)$, with parametric dependence

on the second factor q , that would define a diffeomorphism $dS: \mathbb{R}^n \times \mathbb{R}^n \rightarrow T^*\mathbb{R}^n$ given by¹:

$$dS(x, q) := (x, d_q S(x)), \quad (1.7)$$

or, in local coordinates, $p_k = \partial S / \partial q^k(x, q)$, by means of which one can replace initial position x and initial momentum p , with initial position x and final position q . Furthermore, it is possible to define a symplectic structure ω on $\mathbb{R}^n \times \mathbb{R}^n$ as follows:

$$\omega := (dS)^* \omega_0 = d((dS)^* \theta_0) = \frac{\partial S}{\partial x^j \partial q^k} dx^j \wedge dq^k, \quad (1.8)$$

where $\theta_0 = p_j dq^j$ is the canonical one form on $T^*\mathbb{R}^n$, and $\omega_0 = d\theta_0 = dp_j \wedge dq^j$ is the canonical symplectic structure on $T^*\mathbb{R}^n$ [15]. Consider the Hamiltonian function $H = \frac{1}{2m}p^2 + V(x)$ on $T^*\mathbb{R}^n$ and its associated Hamiltonian vector field X_H defined by the condition $i_{X_H} \omega_0 = dH$, then, when there exists a complete solution S of Hamilton-Jacobi equation, it is possible to define the vector field

$$\tilde{X}_H = ((dS)^{-1})_* X_H \quad (1.9)$$

which is the image under the push-forward of the diffeomorphism $(dS)^{-1}$ (see Eq. (1.7)) of the Hamiltonian vector field X_H . The vector field \tilde{X}_H will be the Hamiltonian vector field, with respect to the symplectic structure ω on the manifold $\mathbb{R}^n \times \mathbb{R}^n$, of the Hamiltonian:

$$\tilde{H} = dS^*(H). \quad (1.10)$$

Since the new variables q^j will be constants of the motion, one gets that:

$$\tilde{X}_H = \frac{\partial S}{\partial x^j} \frac{\partial}{\partial x^j}. \quad (1.11)$$

In order to solve Eq. (1.3) it is better to rewrite it in a more useful form. If one multiplies both sides of the equation by $2A$ the following expression comes to be valid:

$$\frac{\partial A^2}{\partial t} + \nabla \cdot \left(A^2 \frac{\nabla S}{m} \right) = 0. \quad (1.12)$$

If one considers a time-independent solution A , the equation above becomes:

$$\nabla \cdot \left(A^2 \frac{\nabla S}{m} \right) = 0. \quad (1.13)$$

¹It is possible to generalize this construction to an arbitrary configuration manifold Q (see for instance [1]). In such case, dS will be a diffeomorphism only on open submanifolds of $Q \times Q$ and T^*Q .

In order to exhibit an explicit solution of this equation let us notice that if a vector field X preserves the volume form $f\Omega$, then the vector field fX preserves the volume Ω (see [16] for a proof). Since:

$$L_X\Omega = (\operatorname{div}X)\Omega, \quad (1.14)$$

the previous result tells that if the divergence of X with respect to the volume form $f\Omega$ is zero, then the divergence of fX with respect to the volume form Ω is zero. It is already known that the vector field \tilde{X}_H is Hamiltonian with respect to the symplectic form ω ; therefore, it preserves the volume form:

$$f\Omega = \det\left(\frac{\partial^2 S}{\partial x^j \partial q^k}\right) dx^1 \wedge dq^1 \wedge \cdots \wedge dx^n \wedge dq^n.$$

It then follows that the vector field $f\tilde{X}_H$ preserves the volume form Ω on $\mathbb{R}^n \times \mathbb{R}^n$, and thus one gets that:

$$\nabla \cdot \left(\det\left(\frac{\partial^2 S}{\partial x^j \partial q^k}\right) \nabla S \right) = 0. \quad (1.15)$$

Consequently, a stationary solution of Eq. (1.3) is given by:

$$A^2 = \det\left(\frac{\partial^2 S}{\partial x^j \partial q^k}\right). \quad (1.16)$$

The existence of a complete solution for the Hamilton-Jacobi equation, however, implies the system to be completely integrable, that is, there must be n independent constants of the motion in involution, which is a very special situation.

Remark 2 *It is clear that (1.4) is a non-linear equation, and thus, the classical limit, understood as $\hbar \rightarrow 0$, has destroyed the linearity of Schrödinger equation. Looking at this situation from the opposite point of view, one could say that the non-linear Hamilton-Jacobi equation becomes linear. Moreover, when we add the amplitude A and unfold the resulting system into a Hilbert-space setting, it becomes completely integrable. Therefore, it could be tempting to say that the “quantization” procedure may be thought of as a possible linearization procedure for a first order partial differential equation represented by the Hamilton-Jacobi equation for S .*

It is readily seen that the classical limit of the Schrödinger equation highly depends on the chosen wavefunction $\psi(x, t)$, since an arbitrary wavefunction $\psi = Ae^{-\frac{i}{\hbar}W}$ needs not to be such that $\frac{\hbar^2}{2m} \frac{\Delta A}{A} \approx 0$. Accordingly, it seems that the information on the “classical limit” of the theory is not contained

in the whole Hilbert space \mathcal{H} , but in families of suitably-defined states. This idea of considering subsystems is at the basis of the so-called reduction procedures, which have been fruitfully employed in the Hamiltonian description of dynamical systems. Indeed, a common situation arising in reduction procedures is precisely the generation of nonlinear dynamics starting from linear ones (see for instance [17], Ch. 7.1-2).

In Classical Mechanics, (pure) states of a system are described as points of a suitable manifold M , usually a phase-space. The observables of the theory are described as a certain class of real-valued functions on M . Of course, if M is a smooth manifold, the observables are described by real-valued smooth functions. The dynamical evolution is described using a one-parameter group γ_t of transformations of M in itself. If M is a smooth manifold, and γ_t is smooth, then there is a (complete) vector field Γ generating γ_t . The fact that γ_t is a one-parameter group is associated with the fact that one requires the evolution of the system to be completely determined once the initial state $m \in M$ is specified.

In Quantum Mechanics, it is possible to immerse a manifold M in the Hilbert space \mathcal{H} of a physical system, for instance, by means of the so-called generalized coherent states. In this way, to every $m \in M$ there corresponds a normalized vector $|m\rangle \in \mathcal{H}$, and it is possible to define real-valued functions on M starting with quantum observables (described by self-adjoint operators), and vice versa. From this point of view, generalized coherent states can be thought of as a double-way bridge between Classical and Quantum Mechanics, for, on the one hand, they can be used as a tool to achieve the quantization of a given classical system, and, on the other hand, they can be used as a tool to “dequantize” a given quantum system [18].

In the remaining part of this section this last perspective will be adopted by implementing a reduction-like procedure of quantum dynamical maps using generalized coherent states. Specifically the following question will be asked: is it possible to immerse M in \mathcal{H} in such a way that a given quantum unitary evolution on \mathcal{H} defines a one-parameter group of transformations of M in itself? Consequently one could look for a classical-like interpretation of the points of M , and thus, for the dynamical system on it arising from the reduction of the quantum dynamical map. In this sense one can interpret the resulting dynamical map as being classical-like. Of course, a complete answer to this question is not easy to give, and thus this section contains only a preliminary discussion in which the conceptual aspects of this project are outlined and the well-known example of the canonical coherent states for the quantum harmonic oscillator is reformulated accordingly.

1.1.1 Weyl systems and generalized coherent states

In the spirit of Dirac correspondence principle, classical Poisson-Brackets on functions on a phase space are replaced by commutators among linear operators on a Hilbert space. In the case of canonical commutation relations (CCRs) $[\mathbf{Q}, \mathbf{P}] = i\hbar\mathbb{I}$, at least one of the linear operators representing positions \mathbf{Q} and momenta \mathbf{P} must be an unbounded operator, leading to problems related to the domain of definition for the CCRs. To handle this problem Weyl proposed to formulate CCRs in terms of group elements rather than algebra generators [19], [20]. Specifically, let (V, ω) be a symplectic Abelian vector group of finite dimension $2n$, that is, a vector space V endowed with a non-degenerate antisymmetric bilinear form ω (symplectic form) invariant under the action of the vector group. Then, in Weyl's approach the CCRs are replaced with a projective unitary representation \mathbf{U} of the symplectic Abelian vector group V , i.e., for any $v, w \in V$, $\mathbf{U}(v), \mathbf{U}(w)$ are unitary operators on a Hilbert space \mathcal{H} such that:

$$\mathbf{U}(v)\mathbf{U}(w)\mathbf{U}(v)^\dagger\mathbf{U}(w)^\dagger = e^{i\omega(v,w)}. \quad (1.17)$$

By selecting a Lagrangian subspace $X \subset V$, i.e., a maximal isotropic subspace, the unitary operators $\mathbf{U}(v)$ corresponding to an irreducible representation of V can be realized as von Neumann's irreducible representation on the Hilbert space $\mathcal{L}^2(X, d\mu)$ of square integrable functions ψ on X with respect to the Lebesgue measure:

$$(\mathbf{U}(v)\psi)(x) = (\mathbf{U}(x, \alpha)\psi)(x) = e^{i\alpha \cdot x}\psi(x + q). \quad (1.18)$$

where the symplectic vector space V is naturally identified with $X \oplus X^* \cong T^*X$ and vectors $v \in V$ can be written as pairs (x, α) with $x \in X$ and $\alpha \in X^*$. It is well-known that the generators \mathbf{Q} of the subgroup $\mathbf{U}(q, 0)$ and the generators \mathbf{P} of the subgroup $\mathbf{U}(0, \alpha)$ satisfy the CCRs on an appropriate domain [21, 22].

Weyl's idea can be generalized to the so-called quantizer-dequantizer formalism [23], in which projective representations of groups are replaced by two maps U, D , called quantizer and dequantizer respectively. Let (M, μ) be a measure space, for instance a topological space with a Borelian measure, and \mathcal{H} a Hilbert space with its associated spaces $\mathcal{L}(\mathcal{H})$ and $\mathcal{U}(\mathcal{H})$ of linear and unitary operators respectively. One defines two maps $U, D: M \rightarrow \mathcal{U}(\mathcal{H})$, by means of which a unitary operator $U(m)$, or $D(m)$, is associated to any point $m \in M$. The map U allows to build operators starting with functions on M , that is, given a function f in M one can define the linear operator:

$$\mathbf{A}_f := \int_M f(m)U(m)d\mu(m), \quad (1.19)$$

with \mathbf{A}_f acting on the vector $|\psi\rangle \in \mathcal{H}$ as

$$\mathbf{A}_f|\psi\rangle := \int_M f(m)(U(m)|\psi\rangle) d\mu(m).$$

Thus $|\psi\rangle$ will be in the domain of \mathbf{A}_f if $\|\mathbf{A}_f|\psi\rangle\| < \infty$. This will be achieved if the map U is strongly continuous, that is for any $|\psi\rangle \in \mathcal{H}$, the map $x \mapsto U(x)|\psi\rangle$ is continuous, and $f \in \mathcal{L}^1(M, d\mu)$. Notice that in such case (notice that the map $x \mapsto U(x)|\psi\rangle$ is not only continuous but bounded $\|U(x)|\psi\rangle\| \leq \|U(x)\|\|\psi\rangle\| = \|\psi\rangle\|$):

$$\|\mathbf{A}_f|\psi\rangle\| \leq \|f\|_{\mathcal{L}^1}\|\psi\rangle\|,$$

and the operator \mathbf{A}_f is bounded. More general measurable maps f will lead to unbounded operators \mathbf{A}_f . Analogously, starting with D and a linear operator \mathbf{A} one can build a function $f_{\mathbf{A}}$:

$$f_{\mathbf{A}}(m) := \text{Tr}(\mathbf{A} D^\dagger(m)). \quad (1.20)$$

Clearly, whenever \mathbf{A} is an unbounded operator, a careful analysis is needed in order to be sure that the trace in the definition of $f_{\mathbf{A}}$ makes sense.

If the maps U, D are such that:

$$\int_M \text{Tr}(D^\dagger(m)U(m')) f(m') d\mu(m') = f(m), \quad (1.21)$$

for any test function f on M , that is

$$\text{Tr}(D^\dagger(m)U(m')) = \delta(m, m'), \quad (1.22)$$

in the sense of distributions, then if $D(m)$ is strongly continuous too, it is readily seen that on test functions:

$$f_{\mathbf{A}_f}(m) = \text{Tr}(D^\dagger(m)\mathbf{A}_f) = \int_M f(m') \text{Tr}(D^\dagger(m)U(m')) d\mu(m') = f(m). \quad (1.23)$$

If one assumes that the map $f_{\mathbf{A}}$ is integrable in M , then the correspondence $\mathbf{A} \mapsto f_{\mathbf{A}}$ is a left-inverse to the correspondence $f \mapsto \mathbf{A}_f$.

Fixing a fiducial normalized state $|0\rangle$ in the Hilbert space \mathcal{H} , the map U allows to immerse M in the Hilbert space \mathcal{H} rather than in the unitary group $\mathcal{U}(\mathcal{H})$ by means of the map $m \in M \mapsto |m\rangle \in \mathcal{H}$ given by:

$$|m\rangle := U(m)|0\rangle. \quad (1.24)$$

In general, one can immerse a classical-like manifold M in the Hilbert space \mathcal{H} by means of an injective immersion $i: M \rightarrow \mathcal{H}$ with no reference to the unitary group $\mathcal{U}(\mathcal{H})$. The two most common features required for this map are weak continuity, that is, the map $m \mapsto \langle \psi | m \rangle$ is continuous for all $|\psi\rangle \in \mathcal{H}$, and the completeness condition:

$$\int_M |m\rangle\langle m| d\mu(m) = \mathbb{I}. \quad (1.25)$$

Given an orthonormal basis $\{|k\rangle\}$ of \mathcal{H} , one has that:

$$|m\rangle = \sum_k \psi_k(m) |k\rangle, \quad (1.26)$$

and the completeness condition implies that the set of functions $\psi_k(m)$ form an orthonormal set in the Hilbert space $\mathcal{L}^2(M, d\mu)$. A set of states $|m\rangle$ satisfying these properties will be called system of generalized coherent states and the triple (M, U, D) a quantizer-dequantizer scheme or a generalized Weyl system.

Remark 3 *This immersion procedure is very similar to what is done in information geometry where a statistical model \mathcal{M} is immersed in the statistical manifold $\mathcal{P}(X)$ of probability distributions on a measure space X (see [24], [25] and references therein). Indeed, one can pullback the Hermitean tensor²:*

$$\mathfrak{h} := \frac{\langle d\psi | d\psi \rangle}{\langle \psi | \psi \rangle} - \frac{\langle d\psi | \psi \rangle \langle \psi | d\psi \rangle}{\langle \psi | \psi \rangle^2} \quad (1.27)$$

on M to obtain a Riemannian and a (pre)symplectic tensor (the real and the immaginary part of the pullback tensor). The Riemannian tensor defined on M in this way can be thought of as the Quantum analogue of Fisher-Rao metric ([26]).

Analogously to what has been done with the maps U, D in Eq.(1.19) and Eq.(1.20), the parametrized family of states $|m\rangle$ may be used to build linear operators starting with functions (Notice that in this situation the operator valued function $m \mapsto |m\rangle\langle m|$ is strongly continuous):

$$f \mapsto \mathbf{A}_f := \int_M f(m) |m\rangle\langle m| d\mu(m), \quad (1.28)$$

and vice versa:

²Note that this tensor is not defined on the null vector. Indeed, it is the pullback to $\mathcal{H}_0 = \mathcal{H} - \{\mathbf{0}\}$ of an Hermitean tensor on the complex projective space $\mathcal{P}(\mathcal{H})$.

$$\mathbf{A} \mapsto f_{\mathbf{A}}(m) := \langle m | \mathbf{A} | m \rangle . \quad (1.29)$$

If the analogue of the biorthogonality condition (1.22) is satisfied, that is:

$$\text{Tr} (|m\rangle\langle m| |m'\rangle\langle m'|) = \delta(m, m') ,$$

then relation (1.23) holds and $f_{\mathbf{A}_f} = f$ if f is integrable.

Notice that $\mathbf{A}_{f+g} = \mathbf{A}_f + \mathbf{A}_g$, and $f_{\mathbf{A}+\mathbf{B}} = f_{\mathbf{A}} + f_{\mathbf{B}}$. Of course, if \mathbf{A} is unbounded, one has to check that the vectors $|m\rangle$ lie in its domain in order for $f_{\mathbf{A}}(m)$ to make sense. In addition, we note that f is real valued if and only if \mathbf{A}_f is symmetric.

The correspondence $\mathbf{A} \mapsto f_{\mathbf{A}}$ allows to use the Lie and Jordan products on self-adjoint linear operators to define a symmetric and a skew-symmetric product on real-valued functions $f_{\mathbf{A}}$. Indeed, let \odot denote the Jordan product:

$$\mathbf{A} \odot \mathbf{B} := \frac{1}{2} (\mathbf{A}\mathbf{B} + \mathbf{B}\mathbf{A}) , \quad (1.30)$$

and let $[[,]]$ denote the Lie product:

$$[[\mathbf{A}, \mathbf{B}]] := -\frac{i}{\hbar} [\mathbf{A}, \mathbf{B}] , \quad (1.31)$$

on pairs of self-adjoint operators. Then, the brackets of the corresponding functions are defined as follows:

$$(f_{\mathbf{A}}, f_{\mathbf{B}}) := f_{\mathbf{A} \odot \mathbf{B}} , \quad \{f_{\mathbf{A}}, f_{\mathbf{B}}\} := f_{[[\mathbf{A}, \mathbf{B}]]} . \quad (1.32)$$

If there exist $n = \dim(M)$ linear operators $\mathbf{A}_1, \dots, \mathbf{A}_n$ such that:

$$df_{\mathbf{A}_1}(m) \wedge df_{\mathbf{A}_2}(m) \wedge \dots \wedge df_{\mathbf{A}_n}(m) \neq 0 \quad \forall m \in M , \quad (1.33)$$

then $\{df_{\mathbf{A}_1}(m), \dots, df_{\mathbf{A}_n}(m)\}$ form a basis of T_m^*M for all $m \in M$ and one can write:

$$G(df_{\mathbf{A}_j}, df_{\mathbf{A}_k}) := (f_{\mathbf{A}_j}, f_{\mathbf{A}_k}) , \quad (1.34)$$

$$\Lambda(df_{\mathbf{A}_j}, df_{\mathbf{A}_k}) := \{f_{\mathbf{A}_j}, f_{\mathbf{A}_k}\} . \quad (1.35)$$

Given f_1, f_2 arbitrary (real-valued) smooth functions on M their differentials can be expanded in terms of the chosen basis:

$$df_1 = \alpha_1^j df_{\mathbf{A}_j} , \quad df_2 = \alpha_2^j df_{\mathbf{A}_j} , \quad (1.36)$$

and thus the following $(2, 0)$ tensors G and Λ can be written as follows:

$$G(df_1, df_2) := \alpha_1^j \alpha_2^k G(df_{\mathbf{A}_j}, df_{\mathbf{A}_k}) , \quad (1.37)$$

$$\Lambda(df_1, df_2) := \alpha_1^j \alpha_2^k \Lambda(df_{\mathbf{A}_j}, df_{\mathbf{A}_k}), \quad (1.38)$$

where the summation on repeated indices is understood. Notice that, the linear extension of 1.34 and 1.35 according to 1.37 and 1.38 does not agree, in general, with the brackets among linear operators, that is, once a choice of $\{df_{\mathbf{A}_1}(m), \dots, df_{\mathbf{A}_n}(m)\}$ is made for all $m \in M$, it could happen that there are linear operators \mathbf{B}, \mathbf{C} such that:

$$G(df_{\mathbf{B}}, df_{\mathbf{C}}) \neq f_{\mathbf{B} \circ \mathbf{C}}, \quad \Lambda(df_{\mathbf{B}}, df_{\mathbf{C}}) \neq f_{[[\mathbf{B}, \mathbf{C}]]}. \quad (1.39)$$

When the submanifold M is considered to be a constraint manifold, this situation is similar to the one considered by Dirac when dealing with constraints ([9]). In the following paragraph (remark 5), when dealing with the coherent states, an explicit example will be presented where this situation is actually realized.

1.1.2 Dynamical maps in the quantizer-dequantizer formalism

Invariant sets of generalized coherent states. Up to now the attention has been focused on the kinematical description of the system with no attention to the dynamical aspect of the theory which, in Quantum Mechanics, is encoded in a strongly continuous one-parameter group \mathbf{U}_t of unitary operators on the Hilbert space of the system. Now, one may wonder whether a quantum dynamical map $t \mapsto \mathbf{U}_t$ induces a flow γ_t on a classical-like manifold M of generalized coherent states. If so, γ_t could be interpreted as a classical-like dynamical flow on M representing the quantum evolution \mathbf{U}_t .

The generalized reduction procedure principle (as discussed for instance in [17], Ch. 7), states that a necessary condition for \mathbf{U}_t to induce a dynamical map γ_t on M is the invariance of the range $\Sigma = i(M)$ of the immersion i as a subset of \mathcal{H} , with respect to \mathbf{U}_t , that is $\mathbf{U}_t(\Sigma) \subseteq \Sigma$. In the generalized coherent states setting this means that, for all $t \in \mathbb{R}$, $m \in M$ there exists $m_t \in M$ such that:

$$\mathbf{U}_t|m\rangle = |m_t\rangle. \quad (1.40)$$

Then, the induced flow γ_t in M is defined as follows:

$$m \mapsto \gamma_t(m) := m_t. \quad (1.41)$$

In general, this reduction procedure would give rise to a non-linear flow on M , although the initial dynamical map \mathbf{U}_t was given by linear operators.

Notice that if γ_t exists, it must be a one-parameter group of transformations of M . Indeed, being $\mathbf{U}_t \mathbf{U}_{-t} = \mathbb{I}$, one naturally has that γ_{-t} is the inverse map of γ_t , and vice versa. This fact has an immediate consequence, that is, the set M cannot be interpreted as a classical-like configuration space, but rather it should be thought of as a classical-like space of states, i.e., a phase-space, representing a subset of quantum states. This follows from the fact that in general the dynamics induced on configuration space are not one-parameter groups of transformations, but just projections of flows on phase spaces. For example, the motion of a particle in Classical Mechanics calls for the introduction of the cotangent bundle of its configuration space in order to describe its dynamics by means of a vector field, which, in turn, gives rise to a one-parameter groups of transformations.

Hence, if one has an invariant set of generalized coherent states $|m\rangle$, $m \in M$, with respect to the quantum dynamical map \mathbf{U}_t , it reduces to a one-parameter group of transformations γ_t of M , and if M is a smooth manifold and the maps γ_t are smooth, then the resulting vector field Γ describing the dynamics on M must be complete. On the contrary, dynamical vector fields in classical Lagrangian and Hamiltonian Mechanics are often not complete because of the presence of singularities. Notice that further reductions of the dynamical system (M, Γ) can happen, as it is often the case, for instance if the original quantum system has a symmetry group and such group acts on M equivariantly.

Hamilton-Jacobi theory can be helpful in finding examples where such a reduction is possible. Indeed when a dynamical system is completely integrable, it admits a description in terms of action-angle variables and the corresponding dynamical flow is a one parameter group of transformations.

Invariance and complete integrability. Suppose that \mathbf{H} is a self-adjoint operator generating the quantum dynamical map $\mathbf{U}_t = e^{-i\frac{\mathbf{H}t}{\hbar}}$. For simplicity it will be assumed that the Hamiltonian operator \mathbf{H} has a purely discrete spectrum and that the flow γ_t exists. Furthermore, again just for the sake of simplicity, it will be assumed that the spectrum $\sigma(\mathbf{H})$ of the Hamiltonian operator is non-degenerate; however, the extension of the argument to the degenerate case presents no conceptual difficulties.

Let $\{|k\rangle\}$ denote a basis of normalized eigenvectors of \mathbf{H} , and $\mathbf{E}_k = |k\rangle\langle k|$ the orthogonal projector associated to the eigenvector $|k\rangle$. Without loss of generality, one can assume that the immersion $i: M \rightarrow \mathcal{H}$ is such that the states $|m\rangle$ are in the domain of \mathbf{H} for all $m \in M$ if \mathbf{H} is an unbounded operator. Concretely, this amounts to say that the coefficients $\psi_k(m) = \langle k|m\rangle$ are such that:

$$f_{\mathbf{H}^2}(m) = \langle m | \mathbf{H}^2 | m \rangle = \sum_k E_k^2 |\psi_k(m)|^2 < +\infty \quad \forall m \in M, \quad (1.42)$$

where E_k denotes the k -th eigenvalue of \mathbf{H} .

Since $[\mathbf{E}_k, \mathbf{U}_t] = 0$ for all k , it follows that $f_{\mathbf{E}_k}$ is a constant of the motion for γ_t :

$$f_{\mathbf{E}_k}(\gamma_t(m)) = \langle m | \mathbf{U}_t^\dagger \mathbf{E}_k \mathbf{U}_t | m \rangle = \langle m | \mathbf{E}_k | m \rangle = f_{\mathbf{E}_k}(m). \quad (1.43)$$

Of course, these functions will not be all functionally independent, however, since there is an infinite number of them, it could be possible to find a subset $f_{\mathbf{E}_{k_1}}, \dots, f_{\mathbf{E}_{k_N}}$ of constants of the motion where N is such that the system is completely integrable. More generally, let \mathcal{C} be the algebra generated by the functions $f_{\mathbf{E}_k}$. Then the vector field Γ whose flow is given by γ_t will project to the space defined by the algebra \mathcal{C} . Now, if the skew-symmetric tensor Λ defined before, see Eq. (1.35), is non-degenerate and its inverse ω defines a closed 2-form, and if the algebra \mathcal{C} has $\frac{1}{2} \dim M$ independent generators, the system Γ will be completely integrable (see for instance [17], Ch. 8).

In order to make this construction more concrete, the paradigmatic example of coherent states, namely, the canonical coherent states of the Harmonic oscillator, will be illustrated. In this case, the standard creation and annihilation operators \mathbf{a}^+ and \mathbf{a} are such that the Hamiltonian operator is $\mathbf{H} = \hbar\omega(\mathbf{a}^+ \mathbf{a} + \frac{1}{2}\mathbb{I})$, and its spectrum is given by $\{\hbar\omega(n + \frac{1}{2})\}$. Canonical coherent states are given by the map:

$$z \mapsto |z\rangle = e^{z\mathbf{a} - \bar{z}\mathbf{a}^\dagger} |0\rangle = e^{-\frac{|z|^2}{2}} \sum_{n=0}^{+\infty} \frac{z^n}{\sqrt{n!}} |n\rangle, \quad (1.44)$$

where $z \in M = \mathbb{C}$, and $|n\rangle$ is the n -th eigenvector of \mathbf{H} . An explicit calculation shows that:

$$\begin{aligned} \mathbf{U}_t |z\rangle &= e^{-i\frac{\omega t}{2}} e^{-\frac{|z|^2}{2}} \sum_{n=0}^{+\infty} \frac{z^n}{\sqrt{n!}} e^{-in\omega t} |n\rangle = \\ &= e^{-i\frac{\omega t}{2}} e^{-\frac{|z|^2}{2}} \sum_{n=0}^{+\infty} \frac{(ze^{-i\omega t})^n}{\sqrt{n!}} |n\rangle = e^{-i\frac{\omega t}{2}} |ze^{-i\omega t}\rangle. \end{aligned} \quad (1.45)$$

Since $e^{-i\frac{\omega t}{2}}$ is an overall phase factor, it bears no physical relevance, and one can dispose of it. Equivalently, one could have started considering the Hamiltonian operator $\hbar\omega \mathbf{a}^\dagger \mathbf{a}$, and a direct consequence would have been:

$$\mathbf{U}_t|z\rangle = |ze^{-i\omega t}\rangle, \quad (1.46)$$

without the overall phase factor.

Remark 4 *The appearance of the overall phase factor $e^{-i\frac{\omega t}{2}}$ suggests that a more geometrical formulation of the reduction procedure outlined here should be performed considering the immersion of M in the complex projective space $\mathcal{P}(\mathcal{H})$ rather than in the Hilbert space \mathcal{H} . Indeed, $\mathcal{P}(\mathcal{H})$ is precisely the space of pure states of Quantum Mechanics, and, according to [27], there is an infinite-dimensional formulation of complete integrability which applies directly to unitary evolutions on $\mathcal{P}(\mathcal{H})$.*

Considering $\hbar\omega\mathbf{a}^\dagger\mathbf{a}$ as Hamiltonian operator, the dynamical evolution of a canonical coherent state is again a canonical coherent state, therefore, the quantum dynamical map associated to the Hamiltonian operator \mathbf{H} gives rise to a classical-like dynamical map γ_t . Since $|z\rangle$ is in the domain of the Hamiltonian for all $z \in \mathbb{C}$, the one-parameter group γ_t is differentiable, and thus, there is a complete vector field Γ generating it.

Writing³ $z = x + ip$, with $x, p \in \mathbb{R}$, one immediately see that:

$$\gamma_t(x, p) = (x \cos(\omega t) + p \sin(\omega t), p \cos(\omega t) - x \sin(\omega t)), \quad (1.47)$$

and it is clear that this is nothing but the dynamical flow of the harmonic oscillator on $M = \mathbb{C} \cong \mathbb{R}^2$ which is a completely integrable system.

The functions $f_{\mathbf{E}_k}$ are constants of the motion for γ_t :

$$f_{\mathbf{E}_k}(x, p) = \hbar\omega e^{-(x^2+p^2)} \frac{(x^2 + p^2)^k}{(k-1)!}. \quad (1.48)$$

Furthermore, the function $f_{\mathbf{H}}$ is well defined for all $z \in \mathbb{C}$ and reads:

$$f_{\mathbf{H}}(x, p) = \hbar\omega(x^2 + p^2). \quad (1.49)$$

This is precisely the functional form of the Hamiltonian function for the classical harmonic oscillator, and, of course, it is a constant of the motion for γ_t . Being $\dim(M) = 2$, there can not be two (or more) functionally independent constants of the motion, and in fact, we have $df_{\mathbf{H}} \wedge df_{\mathbf{E}_j} = df_{\mathbf{H}} \wedge df_{\mathbf{E}_k} = df_{\mathbf{E}_k} \wedge df_{\mathbf{E}_j} = 0$ for all k, j .

It will be shown now that, in this case, γ_t is the flow of the Hamiltonian vector field Γ associated with $f_{\mathbf{H}}$ by means of the symplectic structure Ω on $M = \mathbb{C} \cong \mathbb{R}^2$ constructed as follows. Consider $\mathbf{X} = \sqrt{\frac{\hbar}{2m\omega}}(\mathbf{a}^\dagger + \mathbf{a})$ and

³Notice that x and p are dimensionless.

$\mathbf{P} = i\sqrt{\frac{\hbar m\omega}{2}}(\mathbf{a}^\dagger - \mathbf{a})$, a direct calculation shows that the real-valued functions $f_{\mathbf{X}}$ and $f_{\mathbf{P}}$ are:

$$f_{\mathbf{X}}(x, p) = \sqrt{\frac{2\hbar}{m\omega}} x, \quad f_{\mathbf{P}}(x, p) = \sqrt{2\hbar m\omega} p, \quad (1.50)$$

and are functionally independent on all \mathbb{C} . The commutation relations associated with \mathbf{X} and \mathbf{P} are $[\mathbf{X}, \mathbf{P}] = i\hbar\mathbb{I}$. Obviously, these commutation relations do not make sense on the whole Hilbert space \mathcal{H} because \mathbf{X} and \mathbf{P} are unbounded operators, however, they do make sense, weakly, on the set of coherent states, that is, $\langle z | [\mathbf{X}, \mathbf{P}] | z \rangle$ is well defined for all z . This means that $\{f_{\mathbf{X}}, f_{\mathbf{P}}\}$ can be computed as follows:

$$\{f_{\mathbf{X}}, f_{\mathbf{P}}\} = \Lambda(df_{\mathbf{X}}, df_{\mathbf{P}}) = 1. \quad (1.51)$$

Consequently one can define the following antisymmetric contravariant tensor on $\mathbb{C} \cong \mathbb{R}^2$:

$$\Lambda = \frac{1}{\hbar} \frac{\partial}{\partial x} \wedge \frac{\partial}{\partial p}. \quad (1.52)$$

It is clear that this is an invertible Poisson tensor. Its inverse Ω is a symplectic form, and reads:

$$\Omega = \hbar dp \wedge dx. \quad (1.53)$$

A straightforward calculation shows that $\Gamma = \Lambda(df_{\mathbf{H}}, \cdot)$ is indeed the vector field generating γ_t . Note that the antisymmetric part Ω' of the pullback to $M = \mathbb{C} \cong \mathbb{R}^2$ of the Hermitean tensor \mathfrak{h} (see Eq. 1.27) is:

$$\Omega' = dp \wedge dx, \quad (1.54)$$

and thus $\Omega = \hbar\Omega'$.

Remark 5 *Going back to (1.39), it is possible now to provide an explicit realization of the situation considered there. At this purpose, let $\mathbf{A} = \frac{1}{2}(|1\rangle\langle 0| + |0\rangle\langle 1|)$ and $\mathbf{B} = \frac{i}{2}(|1\rangle\langle 0| - |0\rangle\langle 1|)$ be two self-adjoint operators. The associated functions are $f_{\mathbf{A}} = e^{-(x^2+p^2)} x$ and $f_{\mathbf{B}} = e^{-(x^2+p^2)} p$. A direct calculation shows that $[[\mathbf{A}, \mathbf{B}]] = \frac{1}{2\hbar} (|0\rangle\langle 0| - |1\rangle\langle 1|)$, and thus*

$$f_{[[\mathbf{A}, \mathbf{B}]]} = \frac{e^{-(x^2+p^2)}}{2\hbar} (1 - x^2 - p^2). \quad (1.55)$$

However, the bracket between $f_{\mathbf{A}}$ and $f_{\mathbf{B}}$ using the Poisson tensor (1.52) is written as follows:

$$\Lambda(df_{\mathbf{A}}, df_{\mathbf{B}}) = \frac{e^{-2(x^2+p^2)}}{2\hbar} (1 - 2x^2 - 2p^2), \quad (1.56)$$

which is different from (1.55). An analogous result holds for $G(df_{\mathbf{A}}, df_{\mathbf{B}})$.

It is interesting to note that the same classical-like dynamical map can be found starting with a Hamiltonian \mathbf{H} having a non-degenerate, purely discrete spectrum with polynomial growth $\sigma(\mathbf{H}) = \{\sum_{j=0}^N \hbar\omega \epsilon_j n^j\}$, that is:

$$\mathbf{H} = \sum_{n=0}^{+\infty} E(n) |n\rangle\langle n|, \quad (1.57)$$

with $E(n) = \sum_{j=0}^N \hbar\omega \epsilon_j n^j$. In order to see this, it is useful to consider the polar form of the immersion map defining the canonical coherent states:

$$|z\rangle = e^{-\frac{\rho}{2}} \sum_{n=0}^{+\infty} \frac{\rho^{\frac{n}{2}}}{\sqrt{n!}} e^{in\varphi} |n\rangle, \quad (1.58)$$

where $z = \sqrt{\rho} e^{i\varphi}$, and deform it as follows⁴:

$$|z\rangle = e^{-\frac{\rho}{2}} \sum_{n=0}^{+\infty} \frac{\rho^{\frac{n}{2}}}{\sqrt{n!}} e^{i(\sum_{j=0}^N \epsilon_j n^j)\varphi} |n\rangle. \quad (1.59)$$

Note that, unlike the case of canonical coherent states for harmonic oscillator Hamiltonian, this immersion presents a discontinuity at $z = 0$. Accordingly, one will consider $M = \mathbb{C}_0 \cong \mathbb{R}^2 - \{(0, 0)\}$.

A straightforward calculation shows that:

$$\mathbf{U}_t|z\rangle = e^{-\frac{\rho}{2}} \sum_{n=0}^{+\infty} \frac{\rho^{\frac{n}{2}}}{\sqrt{n!}} e^{i(\sum_{j=0}^N \epsilon_j n^j)(\varphi - \omega t)} |n\rangle \equiv |z_t\rangle, \quad (1.60)$$

which means that the set of coherent states is invariant with respect to the quantum dynamical map generated by \mathbf{H} . Writing $z = x + ip$, it follows that:

$$\gamma_t(x, p) = (x \cos(\omega t) + p \sin(\omega t), p \cos(\omega t) - x \sin(\omega t)), \quad (1.61)$$

which is again the dynamical flow of the harmonic oscillator (on $M \cong \mathbb{R}^2 - \{(0, 0)\}$).

⁴A slightly more general set of coherent states of this form were investigated in [28].

The function $f_{\mathbf{H}}$ reads:

$$\begin{aligned} f_{\mathbf{H}}(x, p) &= \langle z | \mathbf{H} | z \rangle = \hbar\omega e^{-\rho} \sum_{n=0}^{+\infty} \frac{\rho^n}{n!} \left(\sum_{j=0}^N \epsilon_j n^j \right) = \\ &= \hbar\omega \sum_{j=0}^N \epsilon_j T_j(\rho) = \hbar\omega \sum_{j=0}^N \epsilon_j T_j(x^2 + p^2), \end{aligned} \quad (1.62)$$

where $T_j(\rho)$ is the j -th Touchard polynomial⁵. It is interesting to notice that the antisymmetric part Ω of the pullback to $M \cong \mathbb{R}^2 - \{(0, 0)\}$ of the Hermitean tensor \mathfrak{h} (see Eq. (1.27)) becomes:

$$\begin{aligned} \Omega &= \left(\sum_{j=0}^N \epsilon_j \frac{\partial}{\partial \rho} T_j(\rho) \right) d\rho \wedge d\varphi = \\ &= \frac{1}{x^2 + p^2} \left(\sum_{j=0}^N \epsilon_j \left(x \frac{\partial}{\partial x} T_j(x^2 + p^2) + p \frac{\partial}{\partial p} T_j(x^2 + p^2) \right) \right) dx \wedge dp, \end{aligned} \quad (1.63)$$

and a direct calculation shows that the dynamical vector field Γ generating γ_t is the Hamiltonian vector field associated with $f_{\mathbf{H}}$ by means of $\hbar\Omega$:

$$\hbar\Omega(\Gamma, \cdot) = df_{\mathbf{H}}. \quad (1.64)$$

From this, one can conclude that, in order to guarantee that the immersed manifold $\Sigma(M)$ is invariant with respect to the different quantum dynamical maps arising from the choice of a specific Hamiltonian \mathbf{H} , one has to carefully select the immersions of $M \cong \mathbb{R}^2 - \{(0, 0)\}$. Once, this is done, one always obtains the same reduced classical-like dynamical map γ_t . However, the function $f_{\mathbf{H}}$ and the antisymmetric part Ω of the pull-back of \mathfrak{h} change in such a way that the vector field Γ generating γ_t is Hamiltonian for $f_{\mathbf{H}}$ with respect to Ω , that is, different quantum dynamical maps lead to alternative Hamiltonian description of the same classical-like dynamics.

However we will not develop further this idea. Indeed this section has been used to illustrate some relationships between Hamilton-Jacobi theory and the Quantum-Classical correspondences, both from a kinematical and

⁵The j -th Touchard polynomial is defined as follows:

$$T_j(x) := e^{-x} \sum_{k=0}^{+\infty} \frac{x^k k^j}{k!}.$$

a dynamical point of view, as exposed in the paper [14]. Next sections, instead, will be devoted to the introduction of variational principles for defining Quantum Dynamics and to the relationship between these formulations and the theory of canonical transformations. More emphasis will be laid on this topics since variational principles will play a fundamental role also in the subsequent chapter.

1.2 Variational Principle in Quantum Mechanics

In the previous section it has been shown a first relation between quantum description of particle mechanics and Hamilton-Jacobi theory when one looks at particular states of the Hilbert space associated with a Quantum mechanical system.

A stronger bond between Hamilton-Jacobi theory and Quantum Mechanics was felt by some of the founders of quantum theory from the very beginning. In particular this link was made evident by those authors who analyzed the role of variational principles in Quantum Mechanics. The pioneering work in this field was the paper written by Dirac [29] in 1933, entitled “The Lagrangian in Quantum Mechanics”. In this paper Dirac proposed a definition of canonical transformations in the quantum setting and showed the analogy between Action functionals in classical mechanics and Green functions in quantum mechanics.

The ideas exposed in this article influenced many theoretical physicists in the following decades. In particular Richard Feynmann testified in his Ph.D. thesis [30] how relevant had been the reading of this work for his “path-integral” formulation of Quantum Mechanics.

Instead a different approach was proposed by Julian Schwinger in the 50’s: he elaborated a formulation of quantum mechanics [31] according to which dynamics is derived from a variational principle, in a way more similar to classical Lagrangian mechanics.

In this section we will present this relation between quantum variational principles and Hamilton-Jacobi theory. After a brief summary of Dirac’s ideas, we will focus on Schwinger variational principle and we will complete the general discussion with a revisitation of some known examples in order to make clearer the exposition.

However before going into the Quantum discussion we will briefly recall the variational principle which is used in the Lagrangian formulation of classical particle mechanics.

Let us consider a single particle in classical mechanics. From a kinematical point of view fields are the trajectories of a particle in a certain configuration space. In the simplest situation the configuration space of the system is a vector space, for instance $\mathbb{R}^3 \times \mathbb{R} = \mathbb{R}^4$, where also time dimension has been added. This choice will be useful in the rest of the thesis where the discussion will focus on relativistic frameworks. A generic trajectory is a differentiable section $\gamma : \mathbb{R} \mapsto \mathbb{R}^4 \times \mathbb{R}$.

The starting point of Lagrangian formulation is the choice of the action functional $S[\gamma]$. In many cases this functional is given in terms of a density function, \mathcal{L} , called the Lagrangian, i.e.

$$S[\gamma] = \int_{\mathbb{R}} \mathcal{L}(\gamma, \dot{\gamma}, s) ds, \quad (1.65)$$

where $\dot{\gamma}$ denotes the differential of the map γ . If one introduces a set of globally defined coordinate functions $\{x^\mu\}$ on \mathbb{R}^4 , the functional (1.65) assumes the more familiar form

$$S[\gamma] = \int_{\mathbb{R}} \mathcal{L}\left(x^\mu, \frac{dx^\mu}{ds}, s\right) ds. \quad (1.66)$$

According to the variational principle, the dynamical trajectories are stationary points of the action functional. The variation of the trajectory by means of a tangent vector field, $\delta\gamma$, gives rise to the equations of motion,

$$\delta S = \int_{\mathbb{R}} \frac{d}{d\lambda} \mathcal{L}\left(x^\mu + \lambda\delta x^\mu, \dot{x}^\mu + \lambda \frac{d}{ds} \delta x^\mu\right) ds = 0, \quad (1.67)$$

where the perturbation of the velocities is the differential of the perturbation along the path.

For a complete set of variations⁶, previous stationarity condition corresponds to the Euler-Lagrange equations

$$\frac{d}{ds} \left(\frac{\partial \mathcal{L}}{\partial \dot{x}^\mu} \right) - \frac{\partial \mathcal{L}}{\partial x^\mu} = 0. \quad (1.68)$$

After this short summary let us move on towards the quantum world.

1.2.1 A tribute to Dirac

In this paragraph we want to briefly recall some precursory observations made by Dirac on the possibility of a Lagrangian formulation of Quantum Mechanics. We think it is worth illustrating these ideas because they influenced all subsequent works on the same subject.

⁶By completeness one is requiring the variations to be able to separate trajectories by the values of functionals.

As above mentioned, the central question posed by Dirac is the possibility of introducing a Lagrangian formulation of Quantum mechanics. The main advantages of such a formulation would be the definition of a variational principle and relativistic invariance, since the Action is a scalar quantity. But in what sense is it possible to define a variational principle in Quantum Mechanics? The answer proposed by Dirac is based on contact transformations: his analysis is aimed at the definition of a quantum analogue of classical contact transformations.

Let us consider a classical Hamiltonian dynamical system described in terms of two independent sets of variables, (q_r, p_r) and (Q_r, P_r) . As already stated in the introduction, a contact transformation intertwining the two different descriptions is generated by a function, say $S(q, Q)$, according to the following formulae:

$$p_r = \frac{\partial S}{\partial q_r} \quad P_r = -\frac{\partial S}{\partial Q_r}. \quad (1.69)$$

On the other hand, in quantum mechanics one can choose two different resolutions of the identity or different bases for the same system, one associated with the spectral decomposition of the operator \hat{q} , the other with the spectral decomposition of \hat{Q} . The transformation function connecting these representations is

$$\langle q|Q \rangle, \quad (1.70)$$

which allows to write operators in a “mixed representation”, i.e.

$$\langle q|\hat{\alpha}|Q \rangle = \int dq' \langle q|\alpha|q' \rangle \langle q'|Q \rangle = \int dQ' \langle Q'|\hat{\alpha}|Q \rangle \langle q|Q' \rangle. \quad (1.71)$$

In the following we will use Dirac bra-ket notation, where $|q\rangle$ denote a vector and $\langle q|Q \rangle$ indicates the scalar product of the two vectors.

According to definition (1.71) one has that:

$$\langle q|\hat{p}_r|Q \rangle = -i\hbar \frac{\partial}{\partial q_r} \langle q|Q \rangle, \quad \langle q|\hat{P}_r|Q \rangle = i\hbar \frac{\partial}{\partial Q_r} \langle q|Q \rangle, \quad (1.72)$$

and

$$\langle q|f(\hat{q})g(\hat{Q})|Q \rangle = f(q)g(Q) \langle q|Q \rangle. \quad (1.73)$$

Last expression can be extended also to “well ordered” functions of the operators q and Q , where the ordering means q on the left and Q on the right. Therefore, if one defines the function $U(q, Q)$

$$\langle q|Q \rangle =: e^{-\frac{i}{\hbar}U(q, Q)}, \quad (1.74)$$

equations (1.72) become

$$\langle q|\hat{p}_r|Q\rangle = -i\hbar\frac{\partial U}{\partial q_r}\langle q|Q\rangle, \quad \langle q|\hat{P}_r|Q\rangle = i\hbar\frac{\partial U}{\partial Q_r}\langle q|Q\rangle, \quad (1.75)$$

which are the operator analogue of a classical contact transformation.

A largely studied generating function is the one associated with the dynamical evolution. It is known [32] that the contact transformation relating the value of the dynamical variable q at time T with its value at any other time t is generated by the action function:

$$S(q_t, q_T) = \int_t^T \mathcal{L}(q(\tau), \dot{q}(\tau))d\tau, \quad (1.76)$$

where the integral is evaluated along a solution of the equations of motions passing through the points q_T and q_t at times T and t respectively. Furthermore \mathcal{L} is the Lagrangian function associated with the chosen dynamical system and \dot{q} denotes the time derivative of the function $q(t)$. Indeed when the action functional is evaluated along a given solution of Euler-Lagrange equations it becomes a function of initial and final generalized positions called Hamilton principal function. Quantum analogue of this function is the generating transformation

$$\langle q_t|q_T\rangle = e^{\frac{i}{\hbar}S(q_t, q_T)} \quad (1.77)$$

intertwining between the representations in which either \hat{q}_t or \hat{q}_T is diagonal. In order to simplify the notation let us define the following function:

$$A_\gamma(t_1, t_2) = e^{\int_{t_1}^{t_2} \mathcal{L}dt},$$

where γ is the path connecting $q(t_1)$ and $q(t_2)$ over which the integral is performed.

If one decomposes the time interval $[t, T]$ into smaller sections $[t, t_1], [t_1, t_2], \dots, [t_m, T]$ the final result is:

$$A_\gamma(t, T) = A_\gamma(t, t_1)A_\gamma(t_1, t_2) \cdots A(t_m, T). \quad (1.78)$$

On the other hand it is also possible to write the generating transformation (1.77) as follows

$$\langle q_t|q_T\rangle = \int dq_1 \langle q_t|q_1\rangle \int dq_2 \langle q_1|q_2\rangle \cdots \int dq_m \langle q_m|q_T\rangle, \quad (1.79)$$

where $|q_i\rangle$ denotes the basis of vector associated with the operator q_{t_i} .

And now the fundamental observation made by Dirac: “... from equation (1.79) we can extract the statement that, if we take specified values for q_t and q_T , then the importance of our considering any set of values for the intermediate q 's is determined by the importance of this set of values in the integration on the right hand side of equation (1.79). If we now make \hbar tend to zero, this statement goes over into the classical statement that, if we take specified values for q_t and q_T , then the importance of our considering any set of values for the intermediate q 's is zero unless this values makes the action function stationary.”

In other words according to the action principle the right hand side of equation (1.78) becomes a two-point function only when one replaces for the q_{t_i} the values which make the action function stationary. The quantum analogue of this evaluation is the integration on the right hand side of equation (1.79), the variational principle being contained in the expression of the intermediate generating transformations and in their contribution to the whole set of integrals. This analogy is strenghtened by the observation that in the limit $\hbar \rightarrow 0$ the main contribution to these integrals come from points which make the action function stationary.

Starting from these ideas Feynmann elaborated his formulation of quantum mechanics where the generating transformation is the central object characterizing a given dynamical system. However, in the next paragraph, we will present a different scheme introduced by Schwinger, where quantum dynamics is obtained according to a variational principle. This approach shares same features with Dirac's paper but the conclusions are completely different.

1.2.2 Schwinger's Variational Principle

As already mentioned, in this paragraph we will illustrate another variational principle which was introduced by Schwinger in his formulation of Quantum Theory in order to get quantum dynamics. During the 50's he used this principle to elaborate his theory of Quantized Fields [10] of which QED is the best known example.

However this principle can be also applied to non relativistic Quantum Mechanics of particles. Indeed, as above stated, it is the dynamical principle of Schwinger's formulation of Quantum Theory [31]. We will not enter into the details of the whole formulation, which would require the introduction of many concepts not related to the topics of this chapter. In this paragraph we will focus only on the variational principle for non relativistic quantum systems. Fields will be described in the subsequent section.

Following Schwinger's discussion, let us consider a quantum system de-

scribed by the set of dynamical variables $\{\hat{q}, \hat{p}\}$ obeying the canonical commutation relations

$$[\hat{q}^a, \hat{p}_b] = i\hbar\delta_b^a. \quad (1.80)$$

Concerning the dynamics, let us suppose that it is generated by a Hermitian Hamiltonian operator $\hat{H}(\hat{q}, \hat{p}, t)$ function of the dynamical variables and the evolution parameter t . Let us consider a representation of canonical commutation relations in a coordinate system where positions \hat{q} are diagonal.

The transformation function connecting position representations at the two extremes of an infinitesimal interval of time is given by

$$\langle q', t + dt | q'', t \rangle = \langle q', t | 1 - \frac{i}{\hbar} \hat{H}(\hat{q}(t), \hat{p}(t), t) | q'', t \rangle \quad (1.81)$$

where dynamical variables $\hat{q}(t), \hat{p}(t)$ evolve according to Heisenberg equations of motion:

$$\frac{d\hat{A}}{dt} = \frac{\partial \hat{A}}{\partial t} - \frac{i}{\hbar} [\hat{A}, \hat{H}], \quad (1.82)$$

\hat{A} denoting any observable of the system.

If one considers the variation of this transformation in response to a variation of all its arguments, i.e. $q', q'', t, t + dt$ ⁷ one gets the following results:

$$\begin{aligned} \delta \langle q', t + dt | &= \frac{i}{\hbar} \langle q', t + dt | \hat{p}_a(t + dt) \delta q^a(t + dt) - \hat{H}(t + dt) \delta(t + dt) \\ \delta | q'', t \rangle &= -\frac{i}{\hbar} \hat{p}_a(t) \delta q^a(t) - \hat{H}(t) \delta(t) | q'', t \rangle \end{aligned}$$

and consequently

$$\begin{aligned} \delta \langle q', t + dt | q'', t \rangle &= \frac{i}{\hbar} \langle q', t + dt | \sum_a (\hat{p}_a(t + dt) \delta q^a(t + dt) - \hat{p}_a(t) \delta q^a(t)) - \\ &\quad - (\hat{H}(t + dt) \delta(t + dt) - \hat{H}(t) \delta(t)) | q'', t \rangle, \end{aligned} \quad (1.83)$$

where every δq^a commutes with the whole set of dynamical variables. In particular if the representation of the commutation relations is irreducible every δq^a is a multiple of the identity.

If now one expands $\hat{p}_a(t + dt)$ and $\hat{H}(t + dt)$ according to Heisenberg equations of motions associated with the operator $\hat{H}(t)$ itself and neglects all terms of order higher than one, the following expression is obtained:

$$\delta \langle q', t + dt | q'', t \rangle = \left\langle q', t + dt | \delta \left[\sum_a (\hat{p}_a(t) (\hat{q}^a(t + dt) - \hat{q}^a(t))) - \hat{H}(t) dt \right] | q'', t \right\rangle. \quad (1.84)$$

⁷Here dt represents an "infinitesimal quantity" rather than a differential form as we have been using up to now.

Therefore one gets that:

$$\delta \langle q', t + dt | q'', t \rangle = \langle q', t + dt | \delta \hat{W} | q'', t \rangle \quad (1.85)$$

where the Hermitian operator $\delta \hat{W}$ is the variation of the operator:

$$\hat{W} = dt \left(\sum_a \hat{p}_a(t) \frac{d\hat{q}^a}{dt} - \hat{H}(t) \right) =: dt \hat{L}(t). \quad (1.86)$$

The composition rule of two consecutive transformations is written in terms of integral kernels as follows:

$$\langle q', t + 2dt | q'', t \rangle = \int d\bar{q} \langle q', t + 2dt | \bar{q}, t + dt \rangle \langle \bar{q}, t + dt | q'', t \rangle. \quad (1.87)$$

Consequently, by using Leibniz rule, one can show the validity of the following expression

$$\delta \langle q', t + 2dt | q'', t \rangle = \langle q', t + 2dt | \delta \hat{W}_{t+dt, t+2dt} | q'', t \rangle + \langle q', t + 2dt | \delta \hat{W}_{t, t+dt} | q'', t \rangle. \quad (1.88)$$

Therefore if one considers a finite time interval $[t_1, t_2]$ the following quantum action principle can be derived:

$$\delta \langle q', t_1 | q'', t_2 \rangle = \frac{i}{\hbar} \langle q', t_1 | \delta \hat{W}_{1,2} | q'', t_2 \rangle \quad (1.89)$$

where

$$\hat{W}_{1,2} = \int_{t_1}^{t_2} dt \hat{L}(t)$$

is the action operator, \hat{L} being the corresponding Lagrange operator. This integral is evaluated along a path $(\hat{q}(t), \hat{p}(t))$ which is solution of the Heisenberg equations of motion associated with the Hamiltonian operator $\hat{H}(t)$ which defines the Lagrange operator $\hat{L}(t)$.

Formula (1.89) expresses Schwinger's Quantum Action Principle, according to which the variation of the transformation function which connects two representations of the same quantum system at different times is given in terms of the variation of an action operator.

Let us remark the fundamental role played by Heisenberg equations of motion: since dynamical variables satisfy these equations one has shown the existence of a action operator satisfying (1.89).

However this is not the end of the story. Indeed it is possible to better characterize the form of the variation of the action, since, once one has chosen

the Hamiltonian operator of the system, the only freedom of change is varying initial or final states. Therefore one has that

$$\delta \langle q', t_1 | = \frac{i}{\hbar} \langle q', t_1 | \hat{G}_1 \quad \delta | q'', t_2 \rangle = -\frac{i}{\hbar} \hat{G}_2 | q'', t_2 \rangle , \quad (1.90)$$

where \hat{G}_1 and \hat{G}_2 are Hermitian operator depending only on the dynamical variables at the respective instant of time. Consequently one can conclude that

$$\delta \langle q', t_1 | q'', t_2 \rangle = \frac{i}{\hbar} \langle q', t_1 | \hat{G}_1 - \hat{G}_2 | q'', t_2 \rangle \quad (1.91)$$

and

$$\delta \hat{W}_{1,2} = \hat{G}_1 - \hat{G}_2 .$$

This is the quantum analogue of the Principle of Stationary Action. By using Schwinger's words : “... *It (the Principle of Stationary Action) asserts that the infinitesimal variation of $W_{1,2}$ -which depends upon the variables at all values of t between t_1 and t_2 - in fact involves only variations at the end points, t_1 and t_2 , and so is stationary with respect to variations at any intermediate time.*”

Here is the difference between Dirac's variational principle and Schwinger's Principle of Stationary Action: even if they consider transformation functions as the quantum analogue of the generating functions for canonical transformations, Dirac interprets the averaged superposition of the whole set of possible intermediate states, written in equation (1.79), as a Quantum variational formulation, whereas Schwinger is more “traditional” suggesting to introduce a Quantum Action operator.

Coming back to the Principle of Stationary Action, it is possible to start from this principle and derive Heisenberg equations and the commutation relations between dynamical variables.

Given a path $\gamma : t \in [t_1, t_2] \rightarrow (\hat{q}^a(t), \hat{p}^a(t))$ one can define the Action operator

$$\hat{W}_{1,2} = \int_{t_1}^{t_2} \left(\sum_a \hat{p}_a d\hat{q}^a - \hat{H} dt \right) .$$

Its infinitesimal variation can be written as follows

$$\begin{aligned} \delta \hat{W}_{1,2} &= \int_{t_1}^{t_2} \left(\sum_a (\delta p_a d\hat{q}^a + \hat{p}_a d\delta q^a) - \delta \hat{H} dt - \hat{H} d\delta t \right) = \\ &= \int_{t_1}^{t_2} \left(\sum_a (\delta p_a d\hat{q}^a - d\hat{p}_a \delta q^a) - \delta \hat{H} dt + d\hat{H} \delta t \right) + \int_{t_1}^{t_2} d \left(\sum_a \hat{p}_a \delta q^a - \hat{H} \delta t \right) , \end{aligned} \quad (1.92)$$

where the last term involves only operators on the boundary.

If one imposes the stationarity of the action with respect to variations in the bulk of the interval $[t_1, t_2]$ the following equation must be valid:

$$\sum_a \left(\delta p_a \frac{d\hat{q}^a}{dt} - \frac{d\hat{p}_a}{dt} \delta q^a \right) + \frac{d\hat{H}}{dt} \delta t = \delta \hat{H}. \quad (1.93)$$

Therefore, if one considers only variation that commute with all the dynamical variables, \hat{q} and \hat{p} , equation (1.93) implies the following set of equations:

$$\begin{aligned} \frac{d\hat{q}^a}{dt} &= \frac{\partial \hat{H}}{\partial p_a} \\ \frac{d\hat{p}_a}{dt} &= -\frac{\partial \hat{H}}{\partial q^a} \\ \frac{d\hat{H}}{dt} &= \frac{\partial \hat{H}}{\partial t} \end{aligned}$$

which are Heisenberg equations of motion. Let us notice that one has varied independently both sets of dynamical variables \hat{q} and \hat{p} . This is called the first order variational principle and in general it produces different equations of motion with respect to the Lagrangian formulation presented at the beginning of this section. Indeed Euler-Lagrange equations of motion are implicit differential equation of second order whereas this first order formulation provides first order differential equations, and the two resulting set of equations can be related when the Legendre transformation between the tangent bundle and the cotangent bundle of the configuration space is invertible.

Coming back to the equation (1.92) the total variation of the action operator can be written as

$$\delta \hat{W}_{1,2} = \hat{G}_1 - \hat{G}_2 \quad (1.94)$$

where

$$\hat{G} = \sum_a \hat{p}_a \delta q^a - \hat{H} \delta t.$$

This operator \hat{G} is the sum of two terms: the first one $\hat{G}_q = \sum_a \hat{p}_a \delta q^a$ is the generator of the translation in q whereas the second term $\hat{G}_t = \hat{H} \delta t$ is the generator of time translations.

Since \hat{G}_q is the generator of spatial translations we have that for any observable \hat{F} , the variation $\delta_q \hat{F}$ assumes the following form

$$\delta_q \hat{F} = \frac{-i}{\hbar} [\hat{F}, \hat{G}_q] \quad (1.95)$$

and consequently

$$\frac{\partial \hat{F}}{\partial q^a} = \frac{-i}{\hbar} [\hat{F}, \hat{p}_a]. \quad (1.96)$$

This implies the following set of commutation relations

$$\frac{\partial \hat{q}^b}{\partial q^a} = \frac{-i}{\hbar} [\hat{q}^b, \hat{p}_a] = \delta_a^b \quad (1.97)$$

which are the canonical commutation relations among \hat{q} and \hat{p} . The other commutation relations

$$[\hat{q}^a, \hat{q}^b] = 0 \quad (1.98)$$

are determined by the choice of the Hilbert space representation.

It is known in classical mechanics that the addition of a total time derivative of a function to the Lagrangian does not affect the equations of motion. A similar result is valid for the corresponding Quantum Action Principle. Indeed if one considers two Lagrange operators, \hat{L} and \bar{L} differing by a total time derivative, i.e.

$$\hat{L} - \bar{L} = \frac{d\hat{w}}{dt} \quad (1.99)$$

the difference between the corresponding Action operator is

$$\hat{W}_{1,2} - \bar{W}_{1,2} = \hat{w}_1 - \hat{w}_2, \quad (1.100)$$

where the right-hand side of previous equation is a quantity defined on the boundary of the time interval. Consequently the bulk variations of the two Action operators are not affected by this change in the Lagrange operator and the Quantum Action Principle is still valid even if there is a change of the generators \hat{G}_1 and \hat{G}_2 . Indeed one gets

$$\hat{G}_i - \bar{G}_i = \delta \hat{w}_i \quad (1.101)$$

which expresses the fact that by adding the time derivative $\frac{d\hat{w}}{dt}$ one has changed the Hilbert space representation by means of a unitary transformation.

For instance let us consider the following pair of Lagrange operators

$$\hat{L}_q - \hat{L}_p = \sum_a \left(\hat{p}_a \frac{d\hat{q}^a}{dt} + \frac{d\hat{p}_a}{dt} \hat{q}^a \right) = \frac{d}{dt} \left(\sum_a \hat{p}_a \hat{q}^a \right) = \frac{d}{dt} \hat{w}. \quad (1.102)$$

If one calls $\hat{G}_q = \sum_a \hat{p}_a \delta q^a$ and $\hat{G}_p = -\delta p^a \hat{q}_a$ the corresponding variations one can obtain the following result:

$$\hat{G}_q - \hat{G}_p = \delta \left(\sum_a \hat{p}_a \hat{q}^a \right) \quad (1.103)$$

and consequently the following equation for the generating transformation $\langle q'|p'\rangle$ can be written:

$$\delta \langle q'|p'\rangle = \frac{i}{\hbar} \left\langle q' \left| \sum_a \hat{q}_a \hat{p}_a \right| p' \right\rangle = \frac{i}{\hbar} \left(\sum_a q'^a p'_a \right) \langle q'|p'\rangle. \quad (1.104)$$

This equation can actually be solved and one obtains the following transformation function:

$$\langle q'|p'\rangle = \frac{1}{(2\pi\hbar)^{n/2}} e^{\frac{i}{\hbar}(\sum_a p'_a q'^a)}, \quad (1.105)$$

where n is the number of \hat{q} operators and the coefficient $\frac{1}{(2\pi\hbar)^{n/2}}$ has been chosen to obtain a unitary transformation.

Remark 6 *A remark is in order now. Indeed the analogy between Schwinger's variational formulation of Quantum dynamics and the theory of contact transformations is evident. Let us consider a time-dependent Hamiltonian dynamical system described in terms of the variables $\{q^a, p_a\}$. The generating function $S(q, Q, t_1, t_2)$ of a contact transformation satisfies the equation:*

$$dS(q, Q, t_1, t_2) = \sum_a p_a dq^a - H(q, p, t_1) dt_1 - \sum_a P_a dQ^a + H(Q, P, t_2) dt_2. \quad (1.106)$$

*This is the analogue of the Principle of Stationary Action. The fact that the variation of the transformation function in equation (1.91) is an operator which depends only on the boundary reflects the classical statement that a canonical transformation may be generated by an exact (if the topology of the space is trivial) one form. Furthermore the fact that the graph of an exact one form is a Lagrangian submanifold of the cotangent bundle $T^*Q \times T^*Q$ with respect to the symplectic form $\omega_1 - \omega_2$, is the classical counterpart of the fact that the variation $\delta\hat{W}_{1,2}$ must be the generator of a unitary transformation and consequently a self-adjoint operator.*

1.2.3 Examples

In this paragraph we will present two well-known examples of quantum dynamics formulated a la Schwinger: free particle and harmonic oscillator. This examples will show more evidently the relation between this description and Hamilton-Jacobi theory.

Let us start from the dynamics of a free particle in a one dimensional vector space, with Hamiltonian operator

$$\hat{H} = \frac{\hat{p}^2}{2m}.$$

According to the Principle of Stationary Action, dynamical variables \hat{q}, \hat{p} evolve following Heisenberg equations of motion. Therefore one has that

$$\begin{aligned}\hat{p}(t) &= \hat{p} \\ \hat{q}(t) &= \hat{q} + \frac{\hat{p}}{m}t.\end{aligned}$$

Equation (1.91) in this case becomes

$$\delta \langle q', t | q'' \rangle = \frac{i}{\hbar} \left\langle q', t \left| \left(\hat{p}(t) \delta q' - \hat{p} \delta q'' - \frac{\hat{p}^2}{2m} \delta t \right) \right| q'' \right\rangle, \quad (1.107)$$

where one has to replace \hat{p} with the solution of the equation of motion, i.e.

$$\hat{p} = \frac{m(\hat{q}(t) - \hat{q})}{t}.$$

Since $[\hat{q}, \hat{q}(t)] = \frac{i\hbar t}{m}$, the final equation is:

$$\begin{aligned}\delta \langle q', t | q'' \rangle &= \frac{i}{\hbar} \left\langle q', t \left| \left(\left(\frac{m(\hat{q}(t) - \hat{q})}{t} \right) (\delta q' - \delta q'') - \frac{m(\hat{q}(t) - \hat{q})^2}{2t^2} \delta t \right) \right| q'' \right\rangle = \\ &= \frac{i}{\hbar} \left\langle q', t \left| \left(\left(\frac{m(\hat{q}(t) - \hat{q})}{t} \right) (\delta q' - \delta q'') - \frac{m(\hat{q}^2(t) + \hat{q}^2 - 2\hat{q}(t)\hat{q})}{2t^2} \delta t + \frac{i\hbar \delta t}{2t} \right) \right| q'' \right\rangle.\end{aligned} \quad (1.108)$$

Therefore one can write the equation above as follows:

$$\frac{\delta \langle q', t | q'' \rangle}{\langle q', t | q'' \rangle} = \frac{i}{\hbar} \delta \left(\frac{m(q' - q'')^2}{2t} + \log \left(\frac{i\hbar}{\sqrt{t}} \right) + \log C \right) \quad (1.109)$$

and the corresponding solution is

$$\langle q', t | q'' \rangle = \frac{C}{\sqrt{t}} e^{\frac{i}{\hbar} \frac{m(q' - q'')^2}{2t}}. \quad (1.110)$$

The constant C is chosen by requiring that

$$\lim_{t \rightarrow 0} \langle q', t | q'' \rangle = \delta(q' - q''), \quad (1.111)$$

so that one gets

$$\langle q', t | q'' \rangle = \sqrt{\frac{m}{2i\pi\hbar t}} e^{\frac{i}{\hbar} \frac{m(q' - q'')^2}{2t}}. \quad (1.112)$$

It is worth noticing that the argument of the exponential is the classical action function of the free motion of a single particle and the amplitude is

proportional to the square root of the determinant of the matrix $A_{jk} = \frac{\partial S}{\partial q'^j \partial q''^k}$. This is related to the particular expression of the Hamiltonian operator: the corresponding Heisenberg equations coincide with Hamilton equations of a free particle on a line.

The other example I want to present is the harmonic oscillator. Hamilton operator in this case is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 \hat{q}^2}{2}$$

and the corresponding equations of motion are:

$$\begin{aligned} \frac{d\hat{q}}{dt} &= \frac{\hat{p}(t)}{2m} \\ \frac{d\hat{p}}{dt} &= -m\omega^2 \hat{q}. \end{aligned}$$

The solutions can be written as follows:

$$\hat{q}(t) = \hat{q} \cos(\omega t) + \frac{\hat{p}}{m\omega} \sin(\omega t) \quad (1.113)$$

$$\hat{p}(t) = \hat{p} \cos(\omega t) - m\omega \hat{q} \sin(\omega t), \quad (1.114)$$

and consequently one has that

$$[\hat{q}, \hat{q}(t)] = \frac{i\hbar}{m\omega} \sin(\omega t).$$

Equation (1.89) in this case becomes:

$$\delta \langle q', t | q'' \rangle = \left\langle q', t | \hat{p}(t) \delta q' - \hat{p} \delta q'' - \hat{H} \delta t | q'' \right\rangle, \quad (1.115)$$

and replacing \hat{p} and $\hat{p}(t)$ for the following expressions coming from the solutions (1.114):

$$\begin{aligned} \hat{p} &= \frac{m\omega}{\sin(\omega t)} (\hat{q}(t) - \hat{q} \cos(\omega t)) \\ \hat{p}(t) &= \frac{m\omega}{\sin(\omega t)} (\hat{q}(t) \cos(\omega t) - \hat{q}) \end{aligned}$$

one obtains the following equation:

$$\frac{\delta \langle q', t | q'' \rangle}{\langle q', t | q'' \rangle} = \frac{i}{\hbar} \delta \left\{ \frac{M\omega}{2 \sin(\omega t)} [(q'^2 + q''^2) \cos(\omega t) - 2q'q''] - i\hbar \log \sqrt{\frac{C\omega}{\sin(\omega t)}} \right\}. \quad (1.116)$$

Therefore the solution of this equation is:

$$\langle q', t | q'' \rangle = \sqrt{\frac{m\omega}{2i\pi\hbar \sin(\omega t)}} e^{\frac{i}{\hbar} \left\{ \frac{M\omega}{2 \sin(\omega t)} [(q'^2 + q''^2) \cos(\omega t) - 2q'q''] \right\}}, \quad (1.117)$$

where the integration constant has been chosen as in the previous example. Once more one can notice that the argument of the exponential is the action function for the classical harmonic oscillator and the amplitude is given by the square root of the determinant of the matrix $A_{jk} = \frac{\partial S}{\partial q'^j \partial q''^k}$.

In the subsequent section we will present the generalization of previous result to the theory of Quantum Fields given by Schwinger. This will give the opportunity of discussing Hamilton-Jacobi theory for Field Theories.

1.3 Quantum Field Theory and Hamilton-Jacobi equation

In this section we will briefly describe Schwinger's variational formulation in Quantum Field Theory [10]. We will not go into the details but we will focus only on the relations between this kind of description and Hamilton-Jacobi theory. We will consider only a scalar field theory over a four dimensional Minkowski spacetime. The generalization to field with internal degrees of freedom can be straightforwardly conceived.

Let us consider a four-dimensional space-time \mathbb{R}^4 and a system of coordinate functions x^μ , with $\mu = 0, \dots, 3$. We choose Minkowski metric with signature $(-1, 1, 1, 1)$. Let us introduce the operator-valued field ⁸ $\phi(x)$. A given state of the Hilbert space on which the operator $\phi(x)$ acts, can be characterized by choosing a complete set of commuting observables which can be constructed from the values of the field $\phi(x)$ on a simultaneity surface, σ , associated with a time function, τ . If one denotes such a state as

$$|\zeta, \sigma\rangle, \quad (1.118)$$

where ζ represent the joint spectrum of a maximally commuting set of observables, it is possible to describe the change of description by means of the transformation function

$$\langle \xi, \sigma_1 | \zeta, \sigma_2 \rangle. \quad (1.119)$$

Particularly interesting is the transformation function

$$\langle \zeta', \sigma_1 | \zeta'', \sigma_2 \rangle \quad (1.120)$$

⁸According to modern algebraic description, quantum fields are operator-valued distribution. However for the scope of this discussion I will not consider these details.

which generates the evolution from the simultaneity surface σ_1 to the surface σ_2 .

According to the Quantum Action Principle (1.89) the infinitesimal variation of this transformation function is equal to the infinitesimal variation of a Hermitian operator, the Action operator

$$W_{1,2} = \int_{\sigma_2}^{\sigma_1} \mathcal{L} dx, \quad (1.121)$$

where the operator \mathcal{L} is the Lagrange operator, function of the dynamical fields and their derivatives. The Principle of Stationary Action states that this variation is the difference of two Hermitian operators defined on the two simultaneity surfaces, i.e.

$$\delta \langle \zeta', \sigma_1 | \zeta'', \sigma_2 \rangle = \frac{i}{\hbar} \langle \zeta', \sigma_1 | F(\sigma_1) - F(\sigma_2) | \zeta'', \sigma_2 \rangle. \quad (1.122)$$

After some computations similar to the ones presented in the previous section one has that

$$\delta W_{1,2} = \int_V \left(\frac{\partial \mathcal{L}}{\partial \phi} - \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial \partial_\mu \phi} \right) \right) d^4x + F(\sigma_1) - F(\sigma_2) \quad (1.123)$$

where V is the volume contained between the two simultaneity surfaces σ_1 and σ_2 . According to the Principle of Stationary Action the volume integral must vanish, providing the equations of motion

$$\frac{\partial \mathcal{L}}{\partial \phi} - \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial \partial_\mu \phi} \right) = 0. \quad (1.124)$$

This shows in a more evident way how equations of motion are actually related to the Lagrange operator, a formalism which fits better with the principles of special relativity.

As far as the operators $F(\sigma)$ are concerned, they depends only on the variation of the simultaneity surface $\delta\sigma$. In a relativistic theory one requires the dynamics to be defined in terms of an action of the Poincaré group \mathcal{P} (this point will be made clearer in a following chapter) and one can choose the carrier space of the theory to be a homogeneous space with respect to this action. In the case of Minkowski space-time one can choose planar surfaces and “rigid” transformations (translations and Lorentz transformations) so that the form of the generator $F(\sigma)$ is expressed as follows

$$F(\sigma) = \int_\sigma d\sigma n_\mu (\pi^\mu \delta\phi + T_\nu^\mu \delta x^\nu), \quad (1.125)$$

where $\pi^\mu = \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)}$ and $T_\nu^\mu = \mathcal{L}\delta_\nu^\mu - \pi^\mu \partial_\nu \phi$ is the stress tensor operator.⁹ As above mentioned the variation δx^ν is made up of two contributions, i.e.

$$\delta x^\nu = \epsilon^\nu - \epsilon_\mu^\nu x^\mu ,$$

and consequently the generator $F(\sigma)$ can be written as the sum of three terms: the first is related to the variation of the value of the field, whereas the other two terms are generated by translations and Lorentz transformations. Therefore one gets

$$F(\sigma) = \int_\sigma d\sigma (n_\mu \pi^\mu \delta \phi) + \left(\epsilon^\nu P_\nu + \frac{1}{2} \epsilon_\mu^\nu J_\nu^\mu \right) , \quad (1.126)$$

where

$$P_\nu = \int_\sigma d\sigma n_\mu T_\nu^\mu , \quad J_\nu^\mu = \int_\sigma d\sigma n_\rho (x^\mu T_\nu^\rho - x^\nu T_\mu^\rho) .$$

These operators form a representation of the Lie algebra \mathfrak{p} of the Poincaré group \mathcal{P} . Furthermore the first term is the generator of the variation of the value of the field at a fixed space time point and from this one derives the following relation:

$$\left[\phi(x), \int_\sigma d\sigma n_\mu \pi^\mu \delta \phi \right] = i\hbar \delta \phi(x) , \quad (1.127)$$

which corresponds to the “equal time” commutation relations:

$$[\phi(x), n_\mu \pi^\mu(x')] = i\hbar \delta(x - x') , \quad (1.128)$$

where the δ distribution is defined on the simultaneity surface σ .

Eventually the Principle of Stationary Action provides the following form for the variation of the action operator

$$\delta W_{1,2} = \frac{i}{\hbar} (F(\sigma_1) - F(\sigma_2)) , \quad (1.129)$$

and the right-hand side of this expression can be ordered in such a way that operators involving fields defined on σ_1 stands on the left. In this way one replaces the previous operator equation with an equation for a new operator \mathcal{W} . In particular one can derive the following equations:

$$\begin{aligned} \frac{\delta}{\delta \phi(\sigma_1)} \mathcal{W} &= n_\mu \pi^\mu(\sigma_1) , & \frac{\delta}{\delta \phi(\sigma_2)} \mathcal{W} &= -n_\mu \pi^\mu(\sigma_2) \\ \delta_\mu^{(1)} \mathcal{W} &= P_\mu(\sigma_1) , & \delta_\mu^{(2)} \mathcal{W} &= -P_\mu(\sigma_2) \\ \delta_{\mu\nu}^{(1)} \mathcal{W} &= J_{\mu\nu}(\sigma_1) , & \delta_{\mu\nu}^{(2)} \mathcal{W} &= -J_{\mu\nu}(\sigma_2) , \end{aligned}$$

⁹For field describing systems with internal spin degrees of freedom this tensor will contain an additional term coming from the transformation of the values of the field $\phi(x)$ under Lorentz transformations.

which can be considered as the Hamilton-Jacobi equations for a Relativistic Quantum Field Theory. Let us remark that the description is fully covariant, in the sense that even if a simultaneity surface has been chosen the results are independent of the particular surface. Furthermore the relativistic description has replaced the Hamilton-Jacobi equation $\frac{\partial W}{\partial t} = H$ with a set of equations involving all the generators of the action of the Poincaré group \mathcal{P} . This is in agreement with the notion of relativistic dynamics given by Dirac in his paper [33].

After obtaining the operator \mathcal{W} one can easily solve the equation for the transformation function

$$\delta \langle \zeta', \sigma_1 | \zeta'', \sigma_2 \rangle = \frac{i}{\hbar} \delta \mathcal{W} \langle \zeta', \sigma_1 | \zeta'', \sigma_2 \rangle , \quad (1.130)$$

and the corresponding solution is given by

$$\langle \zeta', \sigma_1 | \zeta'', \sigma_2 \rangle = e^{\frac{i}{\hbar}(\mathcal{W})} . \quad (1.131)$$

Therefore this formulation provides as solution the integrated dynamics, that is the unitary transformation which connects two different configuration of the dynamical variables.

It would be desirable to understand if it is possible to generalize the simple presentation given in these sections to less trivial geometrical situations. For instance it would be very interesting the application to abelian and non-abelian gauge theories, also in the case of a discretized spacetime. Such an application would have deep connections with the developments of quantum simulation techniques [34, 35].

Free Scalar Field As an example let us consider the free Lagrangian of the Klein-Gordon field, $\phi(x)$, which is:

$$\mathcal{L} = \frac{1}{2} (\partial_\mu \phi(x) \partial^\mu \phi(x) - m^2 \phi^2(x)) . \quad (1.132)$$

Stationary points of this Action are solutions of the Klein-Gordon equation

$$(\partial_\mu \partial^\mu + m^2) \phi(x) = 0 . \quad (1.133)$$

If one chooses as time function the coordinate function $x^0 = t$ one can write a solution of the previous equation as follows:

$$\phi(\mathbf{x}, t) = \int_{\mathbb{R}^3} d^3\mathbf{k} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sin(\omega_{\mathbf{k}}T)} \left(\hat{\phi}_{\sigma_1}(\mathbf{k}) \sin(\omega_{\mathbf{k}}(T-t)) + \hat{\phi}_{\sigma_2}(\mathbf{k}) \sin(\omega_{\mathbf{k}}t) \right) , \quad (1.134)$$

where $\hat{\phi}_{\sigma_1}(\mathbf{k})$ is an operator valued field associated with the Fourier transform of the boundary data $\phi(\mathbf{x}, t = 0)$ whereas $\hat{\phi}_{\sigma_2}(\mathbf{k})$ is related to the Fourier transform of the other boundary data $\phi(\mathbf{x}, t = T)$. One can immediately notice that for a given \mathbf{k} there is a corresponding mode oscillating with \mathbf{k} -dependent frequency $\omega_{\mathbf{k}}^2 = |\mathbf{k}|^2 + m^2$ and the operators $\hat{\phi}_{\sigma_1}(\mathbf{k})$ and $\hat{\phi}_{\sigma_2}(\mathbf{k})$ behave analogously to the operators $x(t = 0)$ and $x(t = T)$ in the example of previous section. Therefore one defines the following commutation relations between these oscillating modes ¹⁰

$$\left[\hat{\phi}_{\sigma_1}(\mathbf{k}), \hat{\phi}_{\sigma_2}(\mathbf{k}') \right] = i\delta^{(3)}(\mathbf{k} + \mathbf{k}') \frac{\sin(\omega_{\mathbf{k}}T)}{\omega_{\mathbf{k}}}. \quad (1.135)$$

Since the simultaneity surfaces are planes orthogonal to the x^0 -axis, the conjugate field operator is $\pi(\mathbf{x}, t) = \partial^0 \hat{\phi}(\mathbf{x}, t)$.

For this scalar field the stress tensor operator $T_{\mu\nu}$ is

$$T_{\mu\nu} = \partial_\mu \phi \partial_\nu \phi - g_{\mu\nu} \mathcal{L}. \quad (1.136)$$

Therefore the Hamiltonian operator

$$H(t) = P_0(t) = \int_{\mathbb{R}^3} (\pi^2(\mathbf{x}, t) + |\nabla \phi|^2(\mathbf{x}, t) + m^2 \phi^2(\mathbf{x}, t)) d^3 \mathbf{x}$$

assumes the following form:

$$\begin{aligned} & \frac{1}{2} \int_{\mathbb{R}^3} d^3 \mathbf{k} \left[\left(\hat{\phi}_{\sigma_1}(\mathbf{k}) \hat{\phi}_{\sigma_1}(-\mathbf{k}) + \hat{\phi}_{\sigma_2}(\mathbf{k}) \hat{\phi}_{\sigma_2}(-\mathbf{k}) \right) \right. \\ & \left. - 2 \hat{\phi}_{\sigma_2}(\mathbf{k}) \hat{\phi}_{\sigma_1}(-\mathbf{k}) - i \frac{\sin(\omega_{\mathbf{k}}T) \cos(\omega_{\mathbf{k}}T)}{\omega_{\mathbf{k}}} \right]. \end{aligned} \quad (1.137)$$

Again one can immediately notice the analogy with a harmonic oscillator: this Hamiltonian is the superposition of harmonic oscillator Hamiltonians with \mathbf{k} -dependent frequencies.

By exploiting the analogy with the harmonic oscillator once more the operator functional \mathcal{W} can be written as follows:

$$\begin{aligned} \mathcal{W} = & -\frac{1}{2} \int_{\mathbb{R}^3} d^3 \mathbf{k} \frac{\omega_{\mathbf{k}}}{\sin(\omega_{\mathbf{k}}T)} \left(\left(\hat{\phi}_{\sigma_1}(\mathbf{k}) \hat{\phi}_{\sigma_1}(-\mathbf{k}) + \hat{\phi}_{\sigma_2}(\mathbf{k}) \hat{\phi}_{\sigma_2}(-\mathbf{k}) \right) \cos(\omega_{\mathbf{k}}T) + \right. \\ & \left. - 2 \hat{\phi}_{\sigma_2}(\mathbf{k}) \hat{\phi}_{\sigma_1}(-\mathbf{k}) \right) + \frac{i}{2} \int_{\mathbb{R}^3} d^3 \mathbf{k} \log \left(\frac{\omega_{\mathbf{k}}}{\sin(\omega_{\mathbf{k}}T)} \right), \end{aligned} \quad (1.138)$$

¹⁰It is possible to derive brackets between fields defined on different simultaneity surfaces following Peierls prescription: this is one of the fundamental ingredients of the so-called covariant formalism and it will be the subject of the following chapters.

and one can notice that the last term in the equation above is the logarithm of the functional determinant of the operator $(D(\mathbf{x}, T))^{-1/2}$, where $D(\mathbf{x}, T)$ is the causal Green function (the definition of this Green function will be given in the second chapter of this thesis):

$$D(\mathbf{x}, T) = \int_{\mathbb{R}^3} d^3\mathbf{x} e^{-i\mathbf{k}\cdot\mathbf{x}} \frac{\sin(\omega_{\mathbf{k}}T)}{\omega_{\mathbf{k}}}. \quad (1.139)$$

Therefore the generating functional for the free dynamics of the scalar field $\phi(\mathbf{x}, t)$ is

$$\langle \phi_2, \sigma_2 | \phi_1, \sigma_1 \rangle = (\det(D(\mathbf{x}, T)))^{-\frac{1}{2}} e^{\frac{i}{\hbar} S(\sigma_1, \sigma_2)} \quad (1.140)$$

where the argument of the exponential is the Action function.

Chapter 2

Covariant Brackets

In this chapter we will revisit the possibility of defining covariant brackets with respect to a given action of the Poincaré group. Usual Hamiltonian formalism requires a splitting of space-time into space and time in order to define canonical commutation relations. However many attempts have been done to introduce a fully covariant formalism based on a Lagrangian function. In this chapter we will present some results related to this approach which have been recently published in two papers [36]-[37].

In the first part we will present a more geometrical description of Peierls Bracket [11], which is based on the definition of an action functional. In particular we will start from the analysis of this bracket for particle mechanics and we will give some examples where there are evident connections with the theory of Hamilton-Jacobi equation.

In the following part we will describe how field theories could be dealt with in this formalism.

In the last part of the chapter we will investigate the possibility of defining a Jacobi bracket which is covariant with respect to a given action of the Poincaré group. Indeed, according to a theorem by Kirillov, the most general antisymmetric bracket which is local in a suitable sense is a Jacobi bracket. As we will try to explain such a choice is compatible with the definition of relativistic dynamics given by Dirac in [33] and we will show also a generalization of Peierls' prescription to introduce a Jacobi brackets based on a Lagrangian formulation [37].

2.1 Peierls Bracket

The quest for a covariant bracket, which does not require a splitting of space-time into space and time to be defined, has been a relevant issue since the

advent of relativity. Such a relativistically covariant description of particles and fields would have been necessary in order to understand how to properly define a covariant quantum theory.

The seminal paper [11] by Peierls in 1952 was actually enlightening from this point of view. His approach was based on a clever use of the action functional which avoids the introduction of a splitting into space and time in order to define commutation relations between fields. Peierls bracket was also employed by DeWitt [12] in his attempt to produce a quantum description of general relativity. In particular he faced the problem of extending the definition of Peierls bracket to Gauge Fields.

In this section we will present some ideas, contained in a recent work by Asorey et al. [36], about the geometrical elements that emerge from a careful analysis of Peierls prescription. We will limit to the case of particle mechanics; field theory will be considered later in this chapter.

2.1.1 Peierls Bracket and Geodesical Motion

Action Functional. Let us start from single particle mechanics. One can deal with particle mechanics as well as with field theories. Indeed in the case of a single particle the fields will be the trajectories in a given configuration space. In the simplest situation this configuration space is a vector space, for instance $\mathbb{R}^3 \times \mathbb{R} = \mathbb{R}^4$, where the additional real line is inserted to define time. A generic trajectory is a differentiable section $\gamma : \mathbb{R} \mapsto \mathbb{R}^4 \times \mathbb{R}$.

The fundamental point in this formulation is the choice of the action functional $S[\gamma]$. It plays a double role: first, it provides us with a set of equations of motion by means of the corresponding variational principle (see section 2 of previous chapter), and on the other hand it allows to define tangent vectors to the space of solutions of the equations of motion. Let us consider the action functional of a particle with only a kinetic term, i.e.

$$S[\gamma] = \frac{m}{2} \int_{\mathbb{R}} g(\dot{\gamma}, \dot{\gamma}) ds, \quad (2.1)$$

where g is the background Riemannian metric of the configuration space, m is the mass of the particle, and $\dot{\gamma}$ denotes the differential of the map γ . If one introduces a set of globally defined coordinate functions $\{x^\mu\}$ on \mathbb{R}^4 , the functional (2.1) assumes the more familiar form

$$S[\gamma] = \frac{m}{2} \int_{\mathbb{R}} g_{\mu\nu}(x^\mu) \frac{dx^\mu}{ds} \frac{dx^\nu}{ds} ds. \quad (2.2)$$

For this Lagrangian function Euler-Lagrange equations (see equation (1.68))

become the geodesic equations

$$\frac{d^2 x^\mu}{ds^2} + \Gamma_{\nu\rho}^\mu \frac{dx^\nu}{ds} \frac{dx^\rho}{ds} = 0, \quad (2.3)$$

where $\Gamma_{\nu\rho}^\mu$ are the Christoffel symbols of the Levi-Civita connection associated with the metric tensor $g = g_{\mu\nu} dx^\mu \otimes dx^\nu$.

Remark 7 *A perturbation of a path is actually a homotopy class of paths and in a more general framework a variational principle can be settled by fixing a fiducial path γ_0 and considering another path in the same homotopy class of the referring one. Since these paths enclose an area, one can define a functional directly in terms of a two form, and provide a variational principle by looking for its stationary points. In other words one is looking for critical values of fluxes. This generalization is very useful when dealing with systems which do not admit an intrinsic Lagrangian formulation, e.g. the motion of an electron in the magnetic field generated by a monopole [38, 39].*

Let us now choose a solution γ_0 of Euler-Lagrange equations which will be the reference point in the space of trajectories. One can use the action S and the set of functionals which are defined on this solution to define a tangent space at this point. Indeed by means of one of these functionals, e.g. A , it is possible to set a new variational principle in terms of the modified action $S' = S + \lambda A$. The new Euler-Lagrange equations are written in a compact form as:

$$(\delta S + \lambda \delta A) [\gamma_A] = 0. \quad (2.4)$$

If one is interested in the description of small perturbations $\delta_A \gamma$ with respect to the reference solution γ_0 , the Euler-Lagrange equations simplify and one obtains the following equations:

$$\frac{\nabla^2}{ds^2} \delta_A x^\nu + R(\delta_A \gamma, \dot{\gamma}_0)^\nu_\mu \dot{x}_0^\mu = g^{\mu\nu} \left[\frac{\partial \mathcal{A}}{\partial x^\mu} - \frac{d}{ds} \left(\frac{\partial \mathcal{A}}{\partial \dot{x}^\mu} \right) \right] \Big|_{\gamma=\gamma_0}, \quad (2.5)$$

where A is expressed in terms of a Lagrangian density \mathcal{A} , i.e. $A = \int \mathcal{A} ds$.

The symbol $\frac{\nabla^2}{dt^2}$ denotes the second covariant derivative along the vector field $\dot{\gamma}_0$, and R is the Riemann curvature, both associated with the Levi-Civita connection. On the l.h.s. we immediately recognize the operator, say \mathcal{J} , which appears in Jacobi equation [40]. It is important to stress that these equations allow to define variations, $\delta_A x^\mu$, which are associated with suitable functionals.

Peierls Brackets: Definition and Geometrical Interpretation. Peierls idea is to proceed by selecting two different solutions of Eq. (2.5), one vanishing at the far past along the trajectory, the other one vanishing in the far future, and then taking their difference. The result is a solution of Jacobi equation with no source. This tangent vector may act as a linear operator on other functionals. The result of this action is called Peierls bracket. If $\delta_A^- x^\mu$ and $\delta_A^+ x^\mu$ denote the required solutions, the Peierls bracket of two functionals A, B is

$$\{A, B\}_P = \int_{\mathbb{R}} (\delta_A^+ x^\mu - \delta_A^- x^\mu) \left[\frac{\partial \mathcal{B}}{\partial x^\mu} - \frac{d}{ds} \left(\frac{\partial \mathcal{B}}{\partial \dot{x}^\mu} \right) \right] \Big|_{\gamma=\gamma_0} ds. \quad (2.6)$$

The solutions $\delta_A^\pm x^\mu$ matching the asymptotic past/future conditions can be expressed in terms of the retarded/advanced Green functions

$$G_\pm^{\nu\mu}(s, s') = (\mathcal{J}_{\mu\nu}^\pm)^{-1}(s, s'), \quad (2.7)$$

where

$$\mathcal{J}_{\mu\nu} = \left(g_{\mu\nu} \frac{\nabla^2}{ds^2} + g_{\mu\sigma} R_{\nu\alpha\beta}^\sigma \dot{x}^\alpha \dot{x}^\beta \right) \Big|_{\gamma=\gamma_0}. \quad (2.8)$$

Indeed, in this case

$$\delta_A^+ x^\nu(s) = \int_{\mathbb{R}} G_+^{\nu\mu}(s, s') \left[\frac{\partial \mathcal{A}}{\partial x^\mu} - \frac{d}{ds} \left(\frac{\partial \mathcal{A}}{\partial \dot{x}^\mu} \right) \right] (s') ds' \quad (2.9)$$

$$\delta_A^- x^\nu(s) = \int_{\mathbb{R}} G_-^{\nu\mu}(s, s') \left[\frac{\partial \mathcal{A}}{\partial x^\mu} - \frac{d}{ds} \left(\frac{\partial \mathcal{A}}{\partial \dot{x}^\mu} \right) \right] (s') ds'. \quad (2.10)$$

One may wonder why one is choosing the difference $\delta_A^+ x^\mu - \delta_A^- x^\mu$ in order to define Peierls brackets. The explanation is simple. Let us consider the following difference:

$$\begin{aligned} & g_{\mu\nu} J_1^\mu \left(\frac{\nabla^2}{ds^2} J_2^\nu + R(J_2, \dot{\gamma}_0)^\nu \dot{x}_0^\rho \right) - g_{\mu\nu} J_2^\mu \left(\frac{\nabla^2}{ds^2} J_1^\nu + R(J_1, \dot{\gamma}_0)^\nu \dot{x}_0^\rho \right) = \\ &= \frac{\nabla}{ds} \left(g_{\mu\nu} J_1^\mu \frac{\nabla}{ds} J_2^\nu - g_{\mu\nu} J_2^\mu \frac{\nabla}{ds} J_1^\nu \right) = \frac{d}{ds} \left(\omega_{\mathcal{L}} \left(\left(J_1, \frac{d}{ds} J_1 \right), \left(J_2, \frac{d}{ds} J_2 \right) \right) \right) \end{aligned} \quad (2.11)$$

where ω_L in the final expression represents a two-form on the tangent bundle $T\mathbb{R}^4$ associated with the Lagrangian density \mathcal{L} which is given explicitly by:

$$\omega_{\mathcal{L}} = \frac{\partial^2 \mathcal{L}}{\partial \dot{x}^\mu \partial \dot{x}^\nu} dx^\mu \wedge dv^\nu + \left(\frac{\partial^2 \mathcal{L}}{\partial \dot{x}^\mu \partial x^\nu} - \frac{\partial^2 \mathcal{L}}{\partial x^\mu \partial \dot{x}^\nu} \right) dx^\mu \wedge dx^\nu.$$

If now one chooses $J_1 = \delta_A^+ x^\mu - \delta_A^- x^\mu$ and $J_2 = \delta_B^+ x^\mu - \delta_B^- x^\mu$, where $\delta_B^+ x^\mu - \delta_B^- x^\mu$ is the solution associated with a second functional B , one obtains

$$g_{\mu\nu} J_1^\mu \left(\frac{\nabla^2}{ds^2} J_2^\nu + R(J_2, \dot{\gamma}_0)^\nu \dot{x}_0^\rho \right) - g_{\mu\nu} J_2^\mu \left(\frac{\nabla^2}{ds^2} J_1^\nu + R(J_1, \dot{\gamma}_0)^\rho \dot{x}_0^\nu \right) = 0. \quad (2.12)$$

Consequently

$$\frac{d}{ds} \left(\omega_{\mathcal{L}} \left(\left(J_1, \frac{d}{ds} J_1 \right), \left(J_2, \frac{d}{ds} J_2 \right) \right) \right) = 0, \quad (2.13)$$

which means that the quantity $\omega_{\mathcal{L}}((J_1, \frac{d}{ds} J_1), (J_2, \frac{d}{ds} J_2))$ is preserved along solutions of the referring equations of the motion.

This result actually expresses a general fact: as it will be shown in the next paragraph, Eq.(2.13) remains valid for every action functional coming from a Lagrangian density not only of the kinetic type. Essentially, it is related to the symmetry of the second variation of the action, and when one has a Lagrangian density it gives rise to the two-form $\omega_{\mathcal{L}}$. After proving this it will be easy to see that the expression in brackets actually coincides with Peierls bracket.

2.1.2 Peierls Bracket for a regular Lagrangian

In the previous paragraph Peierls bracket has been introduced and a first application to geodesical motion has been showed. In this paragraph we will extend previous results to the case of a regular¹ Lagrangian \mathcal{L} .

Let us start from a regular Lagrangian function \mathcal{L} on $T\mathbb{R}^N$ and let us introduce a set of coordinate functions $\{x^j, v^j\}$ on $T\mathbb{R}^N$, with $j = 1, 2, \dots, N$. Euler-Lagrange equations (1.68) can be written as:

$$\frac{\partial^2 \mathcal{L}}{\partial v^j \partial v^k} \ddot{x}^k + \frac{\partial^2 \mathcal{L}}{\partial v^j \partial x^k} \dot{x}^k - \frac{\partial \mathcal{L}}{\partial x^j} = 0. \quad (2.14)$$

Concerning the second variation, when the action is written in terms of a Lagrangian density \mathcal{L} the generalization of the operator $\mathcal{J}_{\mu\nu}$ in eq.(2.8) is the following operator $L_{\mu\nu}$:

$$\left(C_{\mu\nu} \frac{d^2}{ds^2} + D_{\mu\nu} \frac{d}{ds} + E_{\mu\nu} \right) \Big|_{\gamma=\gamma_0}, \quad (2.15)$$

¹A Lagrangian function \mathcal{L} on $T\mathbb{R}^N$ is regular if and only if the determinant of the matrix $\frac{\partial^2 \mathcal{L}}{\partial v^j \partial v^k}$ is nowhere vanishing, where (x^j, v^j) denote a set of coordinate functions on $T\mathbb{R}^N$.

which is a linear second order differential equation which acts on a variation $J^\mu(s)$. This operator is written in terms of the following matrices

$$C_{\mu\nu} = -\frac{\partial^2 \mathcal{L}}{\partial \dot{x}^\mu \partial \dot{x}^\nu} \quad (2.16)$$

$$D_{\mu\nu} = -\frac{d}{ds} \frac{\partial^2 \mathcal{L}}{\partial \dot{x}^\mu \partial \dot{x}^\nu} - \frac{\partial^2 \mathcal{L}}{\partial \dot{x}^\mu \partial x^\nu} + \frac{\partial^2 \mathcal{L}}{\partial x^\mu \partial \dot{x}^\nu} \quad (2.17)$$

$$E_{\mu\nu} = -\frac{d}{ds} \frac{\partial^2 \mathcal{L}}{\partial \dot{x}^\mu \partial x^\nu} + \frac{\partial^2 \mathcal{L}}{\partial x^\mu \partial x^\nu} \quad (2.18)$$

evaluated along the reference solution γ_0 .

Since the matrix $C_{\mu\nu}$ is invertible, Euler-Lagrange equations define the following second order vector field [41] Γ on the tangent bundle of the configuration space $T\mathbb{R}^N$:

$$\Gamma = v^j \frac{\partial}{\partial q^j} + F^j \frac{\partial}{\partial v^j}, \quad (2.19)$$

where $F^j = -(C^{-1})^{jk} \left(-\frac{\partial^2 \mathcal{L}}{\partial v^k \partial x^l} v^l + \frac{\partial \mathcal{L}}{\partial x^k} \right)$.

If one considers the tangent lift [41] Γ^\uparrow of the vector field Γ one gets the following vector field on $TT\mathbb{R}^N$:

$$\Gamma^\uparrow = v^j \frac{\partial}{\partial q^j} + F^j \frac{\partial}{\partial v^j} + u_v^j \frac{\partial}{\partial u_x^j} + W^j \frac{\partial}{\partial u_v^j}, \quad (2.20)$$

where $W^j = (C^{-1})^{jk} (D_{kl} u_v^l + E_{kl} u_q^l)$ and we have used the following set $\{x^j, v^j, u_x^j, u_v^j\}$ of coordinate functions on $TT\mathbb{R}^N$.

Now let us consider a variation along a curve γ . A variation $J^k(s)$ can be identified with a vector field along the curve γ and so with a curve $\tilde{\gamma}(s) = (x^k(s), J^k(s))$ on the tangent bundle $T\mathbb{R}^N$. The tangent lift $t\tilde{\gamma}(s) = \left(x^k(s), J^k(s), \frac{dx^k}{ds}(s), \frac{dJ^k}{ds}(s) \right)$ therefore is a curve on the double tangent bundle $TT\mathbb{R}^N$.

On the double tangent bundle there exists a natural transformation, called canonical flip $\phi : TT\mathbb{R}^N \rightarrow TT\mathbb{R}^N$, which is based on the fact that it is possible to introduce two different vector bundle structures on the tangent bundle TE of any vector bundle E over a manifold \mathcal{M} [42]. Specializing this transformation to the case in analysis one can write the following map:

$$\phi(x, v, u_x, u_v) = (x, u_x, v, u_v). \quad (2.21)$$

Applying this transformation to the curve $t\tilde{\gamma}$ one gets the following curve

$$\phi(t\tilde{\gamma})(s) = \left(x^k(s), \frac{dx^k}{ds}(s), J^k(s), \frac{dJ^k}{ds}(s) \right), \quad (2.22)$$

which is an integral curve for the vector field Γ^\dagger if and only if $\gamma(s) = (x^k(s))$ is a solution of the Euler-Lagrange equations (1.68) and $\{J^k(s)\}$ is a solution of the equations (2.15).

Let us now consider the curve $t\tilde{\gamma}(s)$. The projection $T(\pi_M)(t\tilde{\gamma}(s)) = (x^k(s), J^k(s))$ defines a vector field V along the curve $\gamma(s)$. At any point of the curve this vector generates a one parameter group of transformations, and consequently this vector field generates a one parameter family of curves, which are in the same homotopy class as $\gamma(s)$. Therefore the tangent lift of this vector field generates a family of curves which are the differential of the previous family of curves. The tangent lift of this vector field is written as

$$V^\dagger = J^\mu(s) \frac{\partial}{\partial x^\mu} + \frac{dJ^\mu}{ds}(s) \frac{\partial}{\partial v^\mu}, \quad (2.23)$$

and its evaluation along the curve of the tangent bundle $(x^k(s), \frac{dx^k}{ds}(s))$ coincide with the curve in equation (2.22).

Let us now consider the following difference

$$\int \int ds ds' \left(J_1^\mu(s) \frac{\delta^2 S}{\delta \gamma^\mu(s) \delta \gamma^\nu(s')} J_2^\nu(s') - \left(\frac{\delta^2 S}{\delta \gamma^\mu(s) \delta \gamma^\nu(s')} J_1^\mu(s) \right) J_2^\nu(s') \right),$$

where the second variation of the action functional is the operator in equation (2.15). A direct computation shows that this difference can be written as a total derivative, that is

$$\begin{aligned} \int \int ds ds' \left(J_1^\mu(s) \frac{\delta^2 S}{\delta \gamma^\mu(s) \delta \gamma^\nu(s')} J_2^\nu(s') - \left(\frac{\delta^2 S}{\delta \gamma^\mu(s) \delta \gamma^\nu(s')} J_1^\mu(s) \right) J_2^\nu(s') \right) = \\ \int ds \frac{d}{ds} \left(\omega_{\mathcal{L}} \left(V_1^\dagger, V_2^\dagger \right) \right), \end{aligned} \quad (2.24)$$

where $\omega_{\mathcal{L}}$ denotes the following two-form on $T\mathbb{R}^4$

$$\omega_{\mathcal{L}} = \frac{\partial^2 \mathcal{L}}{\partial \dot{x}^\mu \partial \dot{x}^\nu} dx^\mu \wedge dv^\nu + \left(\frac{\partial^2 \mathcal{L}}{\partial \dot{x}^\mu \partial x^\nu} - \frac{\partial^2 \mathcal{L}}{\partial x^\mu \partial \dot{x}^\nu} \right) dx^\mu \wedge dx^\nu. \quad (2.25)$$

Let us introduce the commutator Green function $\tilde{G}^{\mu\nu}(s, s') = G_+^{\mu\nu}(s, s') - G_-^{\mu\nu}(s, s')$. If $J_1(s) = \tilde{G}(\delta A)^2$ and $J_2(s) = \tilde{G}(\delta B)$, where A and B are two functionals of the curve $\gamma^\mu(s)$, the integrand in equation (2.24) is a constant of the motion.

²The expression $\tilde{G}(\delta A)$ will represent the integral $\int \tilde{G}^{\mu\nu}(s, s') \frac{\delta A}{\delta \gamma^\nu}(s') ds'$, where A is a functional of the curve $\gamma^\mu(s)$.

Then it has to be shown that actually this conserved quantity coincides with Peierls bracket. Before this, however, let us introduce another definition of Peierls bracket:

$$\{A, B\}_P = \int_{\mathbb{R}} \delta_A^- x^j \left(\frac{\partial \mathcal{B}}{\partial x^j} - \frac{d}{ds} \left(\frac{\partial \mathcal{B}}{\partial \dot{x}^j} \right) \right) ds - \int_{\mathbb{R}} \delta_B^- x^j \left(\frac{\partial \mathcal{A}}{\partial x^j} - \frac{d}{ds} \left(\frac{\partial \mathcal{A}}{\partial \dot{x}^j} \right) \right) ds. \quad (2.26)$$

This definition and the one in Eq. (2.6) coincide when the action of the variation $\delta_A^+ x^\mu$ over the functional B equals the action of the variation $\delta_B^- x^\mu$ over the functional A [12].

Replacing $J_1 = \delta_A^- x^\mu = G^-(\delta A)$ and $J_2 = \delta_B^- x^\mu = G^-(\delta B)$ in Eq.(2.11), we get

$$\langle \delta B, G^-(\delta A) \rangle (s) - \langle \delta A, G^-(\delta B) \rangle (s) = \frac{d}{ds} \left(\omega_{\mathcal{L}} (G^-(\delta A), G^-(\delta B)) \right). \quad (2.27)$$

Integrating both sides of the equation along the reference path, one gets

$$\{A, B\}_P = \lim_{s \rightarrow -\infty} \omega_{\mathcal{L}} (G^-(\delta A), G^-(\delta B)) (s), \quad (2.28)$$

which does coincide with the previous conserved quantity because in the remote past the effect of the solution $\delta_A^+ x^\mu$ is negligible. Since these expressions coincide one can actually compute the conserved quantity at any point of the trajectory using the variations written in terms of commutator Green function $\tilde{G}(\delta A), \tilde{G}(\delta B)$.

Let us now look at the homogeneous part of the linearized problem (2.15). Since it is a linear differential equation, the space of its solutions is a vector space. As it is a second order ordinary differential equation, the dimension of this vector space is $2 \times 4 = 8$, where 4 is the dimension of the configuration space. One can find a basis of this space by looking for a set of 8 independent solutions. For instance a set of independent solutions are obtained by solving the eight homogeneous differential equations

$$L_{\mu\nu} J_-^\nu = 0 \quad (2.29)$$

$$J_-^{(\rho)}(-T) = J_-^\rho \quad (2.30)$$

$$J_-^{(\rho)}(T) = 0 \quad (2.31)$$

and

$$L_{\mu\nu} J_+^\nu = 0 \quad (2.32)$$

$$J_+^{(\rho)}(T) = J_+^\rho \quad (2.33)$$

$$J_+^{(\rho)}(-T) = 0 \quad (2.34)$$

where the vectors J_+^ρ and J_-^ρ have only one non-vanishing component in the ρ -position with value 1.

In terms of these solutions the Green's function $\tilde{G}^{\mu\nu}(s, s')$ can be written as

$$\tilde{G}^{\mu\nu}(s, s') = \sum_{\rho} \frac{J_+^{(\rho)\mu}(s)J_-^{(\rho)\nu}(s') - J_-^{(\rho)\mu}(s)J_+^{(\rho)\nu}(s')}{W(J_+^{(\rho)}, J_-^{(\rho)})} \quad (2.35)$$

where $W(J_+^{(\rho)}, J_-^{(\rho)}) = \omega_{\mathcal{L}}(J_+^{(\rho)}, J_-^{(\rho)})$ is a constant of the motion.

This choice of variations is actually a choice of a basis of the tangent space to the reference solution γ_0 , seen as a solution of a second order differential equation. This basis will be denoted by $\left\{ \frac{\partial}{\partial x_+^\rho}, \frac{\partial}{\partial x_-^\rho} \right\}$, where x_+ and x_- are the parameters labelling the particular solution.

If now one replaces this expression in the definition of $\delta_A^+ x^\mu - \delta_A^- x^\mu$ the following result is obtained:

$$\delta_A^+ x^\mu - \delta_A^- x^\mu = \sum_{\rho} \frac{J_+^{(\rho)\mu}(s) \int_{\mathbb{R}} J_-^{(\rho)\nu}(s') \frac{\delta A}{\delta x^\nu}(s') ds' - J_-^{(\rho)\mu}(s) \int_{\mathbb{R}} J_+^{(\rho)\nu}(s') \frac{\delta A}{\delta x^\nu}(s') ds'}{W(J_+^{(\rho)}, J_-^{(\rho)})},$$

and its action over a functional B can be written as

$$\begin{aligned} \{A, B\}_P &= \sum_{\rho} \frac{1}{W(J_+^{(\rho)}, J_-^{(\rho)})} \left(\int_{\mathbb{R}} \frac{\delta B}{\delta x^\mu}(s) J_+^{(\rho)\mu}(s) ds \right) \left(\int_{\mathbb{R}} J_-^{(\rho)\nu}(s') \frac{\delta A}{\delta x^\nu}(s') ds' \right) \\ &\quad - \sum_{\rho} \frac{1}{W(J_+^{(\rho)}, J_-^{(\rho)})} \left(\int_{\mathbb{R}} \frac{\delta B}{\delta x^\mu}(s) J_-^{(\rho)\mu}(s) ds \right) \left(\int_{\mathbb{R}} J_+^{(\rho)\nu}(s') \frac{\delta A}{\delta x^\nu}(s') ds' \right). \end{aligned}$$

One can identify variations along a path with the restriction of a vector field along solutions, so that this bilinear operation on functionals can be represented in terms of the bivector field along the space of solutions

$$\Lambda = \sum_{\rho} \frac{1}{W(J_+^{(\rho)}, J_-^{(\rho)})} \frac{\partial}{\partial x_+^\rho} \wedge \frac{\partial}{\partial x_-^\rho}. \quad (2.36)$$

From this expression one can conclude that Peierls bracket is a bilinear antisymmetric operation. However, this does not guarantee that it defines a Poisson structure.

In summary, it has been shown that Peierls bracket can be read actually as a bivector field defined on the space of solutions of a system of differential equations in the case of single particle mechanics. Moreover if the dynamics is covariant with respect to the action of the Poincaré group, this action is directly implemented as a symmetry of the system because it maps solutions into solutions.

Example. Let us consider a very simple example in order to make these ideas clearer.

Let us start with the geodesic motion in a flat Euclidean space, \mathbb{R}^4 . The Euler-Lagrange equations are

$$\delta_{jk} \frac{d^2}{ds^2} x^k = 0 \quad (2.37)$$

and the operator \mathcal{J} in the corresponding Jacobi equation Eq.(2.5) reduces to

$$\mathcal{J} = \delta_{lk} \frac{d^2}{ds^2} J^k. \quad (2.38)$$

Let us consider now a path which is solution of the variational problem and which passes through two established points:

$$x^j(s) = \frac{x_-^j + x_+^j}{2} + \frac{x_-^j - x_+^j}{2T} s. \quad (2.39)$$

The integration constants have been chosen to match the conditions

$$x(-T) = x_- \quad (2.40)$$

$$x(T) = x_+. \quad (2.41)$$

As previously illustrated one has to add a source term to the Jacobi equation (2.5) and then to find two particular solutions, one vanishing in the far past and one in the far future. These two solutions are respectively obtained by convolution with the advanced and retarded Green's functions given by

$$G_+^{jk}(s-s') = \delta^{jk} \theta(s-s')(s-s') \quad (2.42)$$

$$G_-^{jk}(s-s') = \delta^{jk} \theta(s'-s)(s'-s). \quad (2.43)$$

Peierls brackets involves the causal Green's function [43]

$$\tilde{G}^{ij}(s, s') = G_+^{ij} - G_-^{ij} = \delta^{ij} (s - s').$$

If one considers a perturbation given in terms of a density function \mathcal{A} one gets that the required difference is

$$(\delta_A^+ x^j - \delta_A^- x^j)(s) = \delta^{jk} \int_{\mathbb{R}} (s-s') \left(\frac{\partial \mathcal{A}}{\partial x^k} - \frac{d}{ds'} \frac{\partial \mathcal{A}}{\partial \dot{x}^k} \right) (s') ds'. \quad (2.44)$$

Thus the Peierls bracket of two functionals, A and B , expressed in terms of two densities \mathcal{A} and \mathcal{B} is

$$\{A, B\}_P = \delta^{jk} \int_{\mathbb{R}} \int_{\mathbb{R}} (s-s') \left(\frac{\partial \mathcal{B}}{\partial x^j} - \frac{d}{ds} \frac{\partial \mathcal{B}}{\partial \dot{x}^j} \right) (s) \left(\frac{\partial \mathcal{A}}{\partial x^k} - \frac{d}{ds'} \frac{\partial \mathcal{A}}{\partial \dot{x}^k} \right) (s') ds ds',$$

and an explicit calculation shows that this expression does coincide with the conserved quantity

$$\omega_{\mathcal{L}} \left(\left(J_1, \frac{d}{ds} J_1 \right), \left(J_2, \frac{d}{ds} J_2 \right) \right) \quad (2.45)$$

when $J_1 = \delta_A^+ x^j - \delta_A^- x^j$ and $J_2 = \delta_B^+ x^j - \delta_B^- x^j$.

Let us now choose a set of independent solutions of the systems (2.31) and (2.34). A straightforward analysis gives

$$J_+^{(j)}(s) = x_+^{(j)}(s + T) \quad (2.46)$$

$$J_-^{(j)}(s) = x_-^{(j)}(s - T) \quad (2.47)$$

where

$$(x_{\pm}^{(j)})^i = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j. \end{cases} \quad (2.48)$$

Since $\omega_{\mathcal{L}}(J_+^{(j)}, J_-^{(j)}) = 2T$ one gets that the bivector field defining the Peierls bracket is

$$\Lambda = \sum_j T \frac{\partial}{\partial x_+^j} \wedge \frac{\partial}{\partial x_-^j}. \quad (2.49)$$

One can immediately recognize that the tensor Λ defines a Poisson bracket. It coincides with the push-forward of the Poisson tensor $\Lambda_{\mathcal{L}} = \omega_{\mathcal{L}}^{-1}$ with respect to the canonical transformation defined by the Hamilton principal function

$$S(x_-, x_+) = \sum_j \frac{(x_+^j - x_-^j)^2}{2T} \quad (2.50)$$

associated with the Lagrangian density generating the equations of motion.

2.2 From Particles to Fields

In this section we will show how previous construction can be extended to field theory. Actually since the formalism we have adopted in the last section is based on the use of curves and variational principles, this generalization is almost straightforward. The main point is the following: one has to replace the one dimensional manifold representing the parametrization of a curve with a higher dimensional manifold. In particular four dimensional manifolds equipped with a Lorentzian metric tensor are of interest for the description of relativistic field theories.

In the following paragraphs we will investigate the features of this covariant description for fields by examining a simple example: relativistic scalar field without interactions. In this way we will present the main geometrical elements without caring of some technicalities which will make more obscure the exposition.

2.2.1 Peierls Bracket and Scalar Field Theory

Let us start from the relativistic description of a free scalar field. A scalar field is a section of the trivializable bundle $\pi : E = \mathbb{R} \times \mathbb{R}^4 \rightarrow \mathbb{R}^4$, i.e. maps from \mathbb{R}^4 with values in \mathbb{R} . The base manifold \mathbb{R}^4 is equipped with the Minkowski metric tensor $g = \eta_{\mu\nu} dx^\mu \otimes dx^\nu$ where the matrix $\eta_{\mu\nu}$ has the following form:

$$\eta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad (2.51)$$

The free dynamics of this field is given in terms of a variational principle, the action functional being

$$S[\phi] = \int_{\mathbb{R}^4} \frac{1}{2} (\eta^{\mu\nu} \partial_\mu \phi \partial_\nu \phi - m^2 \phi^2) d^4x = \int_{\mathbb{R}^4} \mathcal{L} d^4x. \quad (2.52)$$

One can immediately see that the Lagrangian density \mathcal{L} is a function defined on the first jet bundle J^1E of the vector bundle E , in particular it is evaluated over the first prolongation $j^1\phi$ of the field ϕ . The first jet bundle generalize the notion of tangent bundle to field theories, replacing the single derivatives of a curve with the whole set of partial derivative of a field, as well as the first prolongation of a field ϕ generalizes the notion of differential $t\gamma$ of a curve γ . More details are contained in the Appendix A.

In this simple example one can introduce a single chart on the first jet bundle J^1E with the following coordinate function $J^1E \ni p \rightarrow (x^\mu, u, u_\mu)$. The first prolongation $j^1\phi$ of a section ϕ of the vector bundle E is a section of the first jet bundle which in the previous coordinates can be written as $j^1\phi(x) = (\phi(x), \partial_\mu \phi(x))$.

Therefore one can write the action functional in equation (2.52) as follows

$$S[\phi] = \int_{\mathbb{R}^4} (j^1\phi)^*(\mathcal{L}) d^4x. \quad (2.53)$$

According to Lagrangian variational principle, one is looking for stationary points of the action functional. A variation can be represented by a

compact support vertical vector field $U = U(x)\frac{\partial}{\partial u}$ along the field ϕ ; actually, since the Lagrangian density involves the first prolongation of the field ϕ , a variation is associated with the first prolongation U^1 of the vertical vector field U . In coordinates one obtains:

$$U^1 = U \frac{\partial}{\partial u} + \frac{dU}{dx^\mu} \frac{\partial}{\partial u_\mu}.$$

Therefore stationary points of the action functional satisfy

$$\delta S_\phi[U] = \int_{\mathbb{R}^4} (j^1\phi)^*(L_{U^1}\mathcal{L})d^4x = 0, \quad (2.54)$$

for every variation U . Euler-Lagrange equation is:

$$\partial_\mu\partial^\mu\phi + m^2\phi = 0. \quad (2.55)$$

In order to apply Peierls prescription one has to select a reference solution ϕ_0 of Euler-Lagrange equation. As already outlined in the previous section one has to introduce a new functional $S' = S + \lambda A$ and considering the linearized Euler-Lagrange equation associated with this new functional around the reference solution ϕ_0 . The result is an equation for a variation $\delta_A\phi$ which can be written in a compact form as follows:

$$\frac{\delta^2 S}{\delta\phi(x)\delta\phi(x')} \delta_A\phi(x') = \frac{\delta A}{\delta\phi(x)}, \quad (2.56)$$

where the second variation of the action is a linear operator evaluated along the solution ϕ_0 . In the case of free dynamics of a scalar field this operator coincides with Klein-Gordon equation since the initial Euler-Lagrange equations were already linear, that is:

$$\frac{\delta^2 S}{\delta\phi(x)\delta\phi(x')} \delta_A\phi(x') = \partial_\mu\partial^\mu\delta_A\phi + m^2\delta_A\phi \quad (2.57)$$

At this point Peierls procedure ends with the selection of a particular solution $\tilde{\delta}\phi_A$ of the equation (2.56) written as the difference

$$\tilde{\delta}\phi_A = G^+(\delta A) - G^-(\delta A) = \tilde{G}(\delta A) \quad (2.58)$$

where $\tilde{G} = G^+ - G^-$ is the commutator or causal Green function associated with the linear equation (2.56). Let us recall once more that this solution is actually a solution of the homogeneous equation associated with equation (2.56).

As already analyzed in the previous section this choice allows to define a vector tangent to the space of solutions at the point ϕ_0 and this tangent vector acts as a differential operator on other functionals, for instance B ; the result of this action is the Peierls bracket which can be written as

$$\{A, B\}_P = \int_{\mathbb{R}^4} \tilde{\delta}\phi_A(x) \frac{\delta B}{\delta\phi(x)} d^4x. \quad (2.59)$$

Let us now consider the difference

$$V(x') \left(\frac{\delta^2 S}{\delta\phi(x')\delta\phi(x)} U(x) \right) - \left(V(x') \frac{\delta^2 S}{\delta\phi(x')\delta\phi(x)} \right) U(x), \quad (2.60)$$

where U, V are two arbitrary variations. Since the second variation is a symmetric operator this difference can be rewritten as a quadridivergence (see [12, 44]). In the case of Klein-Gordon equation one obtains the following result:

$$V(x) (\partial_\mu \partial^\mu U(x)) - (\partial_\mu \partial^\mu V(x)) U(x) = \partial^\mu (V(x) (\partial_\mu U(x)) - (\partial_\mu V(x)) U(x)), \quad (2.61)$$

and when the two variations U, V are solutions of the homogeneous equations associated with equation (2.56) one obtains that this divergence is zero. If now one integrates the right hand side of last equation over a volume contained between two simultaneity surfaces (these surfaces can be selected by defining a time function on \mathbb{R}^4) one can see that the value of the integral does not depend on the chosen surface and this integral defines a two-form on the space of fields solutions of Klein-Gordon equation. It is possible to write this form in a more effective way as follows:

$$\Omega_\phi^\Sigma[U, V] = \int_\Sigma i_\Sigma^* (n^\mu (V(x) (\partial_\mu U(x)) - (\partial_\mu V(x)) U(x))) d\sigma, \quad (2.62)$$

where i_Σ^* is the pullback through the immersion of the simultaneity surface Σ in \mathbb{R}^4 and $d\sigma$ is the measure on the surface Σ induced by the measure on \mathbb{R}^4 .

In order to make more evident the generalization to other field theories one can write this bracket in terms of tensors on the first jet bundle. Indeed every first jet bundle possesses a vector valued m -form S which in coordinates can be written as

$$S = (du - u_\mu dx^\mu) \wedge (i_{\partial_\nu} \omega) \otimes \frac{\partial}{\partial u_\nu}, \quad (2.63)$$

where ω is a volume form on \mathbb{R}^4 . The contraction of this vector valued m -form with the differential one form $d\mathcal{L}$ gives rise to a (m) -form on the

first jet bundle which one calls $d_S\mathcal{L}$. In coordinates it assumes the following expression

$$d_S\mathcal{L} = \frac{\partial\mathcal{L}}{\partial u_\nu}(du - u_\mu dx^\mu) \wedge (i_{\partial_\nu}\omega). \quad (2.64)$$

The differential of this m -form is a $(m+1)$ -form on the first jet bundle which can be contracted with two variations, i.e. two vertical vector fields, in order to obtain a $(m-1)$ -form. The pullback of this $(m-1)$ -form through the prolongation $j^1\phi$ of a solution of Euler-Lagrange equations is a $(m-1)$ -form on the base manifold \mathbb{R}^4 which can be integrated on a surface Σ . Since ϕ is a solution of Euler-Lagrange equations this integral does not depend on the chosen surface and defines a two-form on the space of solutions. Therefore the expression (2.62) can be rewritten in an intrinsic way as follows:

$$\Omega_\phi^\Sigma[U, V] = \int_\Sigma i_\Sigma^*(j^1\phi)^*(i_V^1 i_U^1 d(d_S\mathcal{L})). \quad (2.65)$$

As already shown in previous section, if one replaces the variations U, V with the variations $\tilde{\delta}\phi_A, \tilde{\delta}\phi_B$ one obtains Peierls bracket. Therefore one can write the following expression:

$$\{A, B\}_P(\phi) = \Omega_\phi^\Sigma[\tilde{\delta}\phi_A, \tilde{\delta}\phi_B]. \quad (2.66)$$

In particular when we specialize to the case of scalar field theory without interaction one can obtain another interesting expression which is associated with a specific choice of a time function.

If one considers the coordinate function x_0 as a globally defined time function τ the level sets of which define simultaneity surfaces, a solution of Klein-Gordon equation whose values at $\tau = \tau_1$ and $\tau = \tau_2$ are given by the two functions $\phi_1(\mathbf{x})$ and $\phi_2(\mathbf{x})$ respectively, is

$$\phi(\mathbf{x}, \tau) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{d\mathbf{k} e^{i\mathbf{k}\mathbf{x}}}{\sin \omega_k(\tau_2 - \tau_1)} \left(\tilde{\phi}_1(\mathbf{k}) \sin \omega_k(\tau - \tau_2) - \tilde{\phi}_2(\mathbf{k}) \sin \omega_k(\tau - \tau_1) \right).$$

This can be seen as the superposition of harmonic oscillators with k -dependent frequencies. The commutator Green function can be written as follows

$$\tilde{G}(x, y) = \int_{\mathbb{R}^3} \frac{d\mathbf{k}}{(2\pi)^3 \omega_k} e^{i\mathbf{k}(\mathbf{x}-\mathbf{y})} (\sin(\omega_k x_0) \cos(\omega_k y_0) - \cos(\omega_k x_0) \sin(\omega_k y_0)).$$

After some lengthy computations one can write the Peierls bracket according to the following formula:

$$\{A, B\}_P = \int_{\mathbb{R}^4} d^4 z \int_{\mathbb{R}^4} d^4 y \int_{\mathbb{R}^3} \frac{d\mathbf{k}}{(2\pi)^3 \omega_k} e^{i\mathbf{k}(\mathbf{y}-\mathbf{z})} \sin(\omega_k(y_0 - z_0)) \frac{\delta A}{\delta \phi}(y) \frac{\delta B}{\delta \phi}(z),$$

which can be seen as the superposition over the modes labelled by \mathbf{k} of Peierls brackets for a harmonic oscillator. Furthermore each one of these modes can be interpreted as the superposition of a forward propagating mode and a backward propagating mode, J_+ and J_- respectively. Causality is respected as can be shown by computing the brackets between the two functionals $\phi(x_1) = \int_{\mathbb{R}^4} \phi(x)\delta(x - x_1)$ and $\phi(x_2) = \int_{\mathbb{R}^4} \phi(x)\delta(x - x_2)$, that is:

$$\{\phi(x_1), \phi(x_2)\}_P = \tilde{G}(x_1 - x_2). \quad (2.67)$$

2.2.2 A final comparison

In the final paragraph of this section we will make a brief comparison between the covariant description of the previous sections and the Hamiltonian covariant description recently elaborated in the paper [44]. This will allow us to clarify the relationship between this description and Hamilton-Jacobi theory seen as the theory of generating functions of canonical transformations.

Let us start from the space of fields. These are sections of a fibre bundle over a $(d + 1)$ -dimensional manifold \mathcal{M} equipped with a metric tensor g . The space of physical states for a system described by a second order partial differential equation are section of the first jet bundle J^1E which are first prolongation $j^1\phi$ of sections ϕ of the fibre bundle E . Let us introduce on J^1E the following coordinate functions $\{x^\mu, u^a, u_\mu^a\}$.

It is possible to equip this space of sections Γ_J with some suitable differential structure (for instance Hilbert spaces if one considers solutions which belong to some Sobolev spaces, but in general this choice will depend on the physical interpretation of the fields). Therefore we will suppose to be able to perform, at least formally, the usual operations of the differential calculus on manifolds.

In order to define an action functional one can introduce the following $(d + 1)$ -form on J^1E which is written by means of the natural vector-valued $(d + 1)$ -form S on the first jet-bundle and a Lagrangian function \mathcal{L} . This form can be written as follows:

$$\theta_{\mathcal{L}} = d_S \mathcal{L} + \mathcal{L}\omega = \frac{\partial \mathcal{L}}{\partial u_\mu^a} du^a \wedge i_{\partial_\mu} \omega - \left(\frac{\partial \mathcal{L}}{\partial u_\mu^a} u_\mu^a - \mathcal{L} \right) \omega, \quad (2.68)$$

whereas the corresponding action functional assumes the following form:

$$S[\phi] = \int_{\mathcal{M}} (j^1\phi)^* \theta_{\mathcal{L}}. \quad (2.69)$$

Variations U of a field ϕ can be identified with a vertical vector field along the field ϕ ; in particular, since the action involves the first prolongation of the

field ϕ the corresponding variation is the first prolongation U^1 of the vertical field associated with U along $j^1\phi$. Critical point of the action functional satisfy the following equation:

$$dS_\phi[U] = 0, \quad (2.70)$$

for a generic variation U . Let us show how to obtain Euler-Lagrange equation in this approach. Indeed one has that

$$\begin{aligned} dS_\phi[U] &= \frac{d}{ds} S[\phi_s]|_{s=0} = \int_{\mathcal{M}} \frac{d}{ds} (j^1\phi_s)^* \theta_{\mathcal{L}}|_{s=0} = \int_{\mathcal{M}} (j^1\phi)^* L_{U^1}(\theta_{\mathcal{L}}) = \\ &= \int_{\mathcal{M}} (j^1\phi)^* i_{U^1} d\theta_{\mathcal{L}} + \int_{\mathcal{M}} (j^1\phi)^* di_{U^1}\theta_{\mathcal{L}}. \end{aligned} \quad (2.71)$$

If the manifold does not have a boundary the second term in the last equality vanishes as a consequence of Stoke's theorem whereas the first term gives Euler-Lagrange equation, as can be seen by a direct computation which gives the following result:

$$(j^1\phi)^* i_{U^1} d\theta_{\mathcal{L}} = -U^a \left(\frac{\partial}{\partial x^\mu} \left(\frac{\partial \mathcal{L}}{\partial u_\mu^a} \right) - \frac{\partial \mathcal{L}}{\partial u^a} \right) \omega. \quad (2.72)$$

Furthermore one can interpret the previous term as the definition of a one-form

$$E\mathcal{L}_\phi[U] = \int_{\mathcal{M}} (j^1\phi)^* i_{U^1} d\theta_{\mathcal{L}}, \quad (2.73)$$

over the space of physical fields and the zeros of this one-form are the solution of Euler-Lagrange equation. We will denote the space of these solutions by \mathcal{EL} .

Let us suppose now that the spacetime admits a time function and let us consider a volume contained between two simultaneity surfaces, Σ_1, Σ_2 . Equation (2.71) restricted to this volume has both a contribution from the bulk and another from the boundary. If one considers only fields which are solutions of Euler-Lagrange equations the bulk contribution vanishes and one gets only the boundary terms, which are:

$$\int_{\mathcal{M}} (j^1\phi)^* di_{U^1}\theta_{\mathcal{L}} = \int_{\Sigma_2} i_{\Sigma_2}^* (j^1\phi)^* (i_{U^1}\theta_{\mathcal{L}}) - \int_{\Sigma_1} i_{\Sigma_1}^* (j^1\phi)^* (i_{U^1}\theta_{\mathcal{L}}) \quad (2.74)$$

where

$$i_{U^1}\theta_{\mathcal{L}} = \frac{\partial \mathcal{L}}{\partial u_\mu^a} U^a i_{\partial_\mu} \omega. \quad (2.75)$$

Equation (2.74) defines a one form $\alpha_{\partial\mathcal{M}}$ on the manifold which is the cartesian product $\mathcal{I}_{\Sigma_1} \times \mathcal{I}_{\Sigma_2}$ of the manifolds corresponding to the boundary values $\{\varphi^a, \pi_a\}$ of the fields ϕ^a and the normal momenta $p_a = n^\mu \frac{\partial \mathcal{L}}{\partial u_\mu^a}$ ³ on the surfaces

³ n^μ denotes the normal vector to the surface under analysis.

Σ_1 and Σ_2 . The differential of this one-form determines a two-form on the same manifold which in general will be only presymplectic. This two-form coincides with the expression in equation (2.65) when evaluated on vertical vector fields. If the Lagrangian is not degenerate the manifold is a symplectic manifold and the space \mathcal{EL} is an isotropic submanifold. If Euler-Lagrange equations give rise to a vector field and its flow determines a one-to-one correspondence between the data on Σ_1 and Σ_2 for any possible choice of the two surfaces Σ_1 and Σ_2 , the vector field is complete and the space \mathcal{EL} is a Lagrangian submanifold of $\mathcal{I}_{\Sigma_1} \times \mathcal{I}_{\Sigma_2}$. Therefore smooth tensors on the space of solutions \mathcal{EL} can be associated to smooth tensors on the space \mathcal{I}_{Σ_1} which can be considered as the manifold of the initial data of the physical fields.

Furthermore, if for any pair of values $\varphi_{\Sigma_1}^a, \varphi_{\Sigma_2}^a$ there is only one solution connecting them, the dynamical system is completely integrable. Therefore smooth tensors on the space of solutions of Euler-Lagrange equations are related to smooth tensors on the product manifold $\mathcal{F} \times \mathcal{F}$ corresponding to the values of the field on the two surfaces Σ_1 and Σ_2 .

After this comparison with the covariant formalism in [44], next section will be devoted to the introduction of a Jacobi bracket on the space of solutions of Euler-Lagrange equations coming from an action functional S with a given Lagrangian density \mathcal{L} . However, before entering into the details, the first paragraph of next section will contain a series of considerations originated from the reading of some enlightening papers which has motivated the subsequent investigation on Jacobi brackets.

2.3 Covariant Jacobi Brackets for Test Particles

2.3.1 Historical Remarks: On Relativistic Forms of Dynamics and Jacobi Brackets

The advent of relativity has forced physicist to think of dynamics in different terms. In the case of special relativity Dirac [33] explains very well what would be a reasonable meaning of relativistic dynamics: the construction of a set of observables closing on the Lie algebra of the Poincaré group. In order to preserve covariance with respect to this group, Dirac suggests to replace the conventional time translation with the full translation subgroup of the Poincaré group and various realizations of the Poincaré algebra are called *forms* of relativistic dynamics.

In modern mathematical language one would say that a form of relativis-

tic dynamics consists in a realization of the abstract commutation relations of the Lie algebra of the Poincaré group as derivations of a certain associative algebra of observables. Notice that this formulation does not discriminate between classical and quantum systems and can be used in both instances. Indeed one of the most relevant achievement of modern mathematics as applied to Physics has been the possibility of using abstract relations to understand and discuss physical laws without using a specific realization. This way of formulate problems allows to separate the aspects which are general from the ones that are related with a chosen realization. For instance the language of abstract algebras is at the base of Dirac's *analogy principle* that allows to relate the quantum description of physical systems and their corresponding classical counterparts.

In a two pages paper Wigner raised the question[45]: to what extent do the equations of motion determine the commutation relations? Adopting Dirac's point of view ,one might rephrase Wigner's problem by searching to what extent the invariance under the Poincaré group would determine the commutation relations.

As the Lie algebra structure is essentially determined by the associative structure which admits the Lie algebra as an algebra of derivations [46],this amounts to ask for all possible associative products which admit as derivations the infinitesimal generators of the Poincaré group. Obviously the answer is not unique: for instance, in the quantum setting the two associative operator products $A \cdot B$ and $A \cdot K \cdot B$ where K is any operator function of the Casimir operator for the Poincaré group, admit the Lie algebra of the Poincaré group as derivations. Nevertheless in both cases these derivations are inner (see Ref. [46]), i.e. they are realized as commutators with an element of the algebra itself. Actually, in the case of the algebra of observables of a quantum mechanical system, all the derivations are inner. However the classical limits (for instance in the sense of Moyal products see Ref. [47]) of these two associative products and of the corresponding commutators have different properties; in the first case the commutator is related to a Poisson bracket, whereas for the second situation the limiting algebra defines a Jacobi bracket.⁴

Therefore in the final section of this chapter it will be shown a possible generalization of the covariant formalism outlined in previous sections by replacing Peierls Bracket with a more general Jacobi Bracket. This idea has been presented in a recent work by Asorey et al. [37]. We will focus on a single example, the Lagrangian describing unparametrized geodesics for

⁴More general in paper [47] it is shown that in presence of KMS states, the classical limit is indeed a Jacobi bracket.

the Minkowski spacetime, but the result can be generalized to the space of geodesics of more general manifolds equipped with a metric tensor.

Before entering this discussion we will start from a digression which will be useful to properly interpret the final result.

2.3.2 Contact Manifolds out of the Klein-Gordon Equation

As above announced in this paragraph we will start with a discussion on the possibility of defining contact structures and Jacobi brackets on physically meaningful submanifolds of the cotangent bundle $T^*\mathbb{R}^4$, where the base manifold \mathbb{R}^4 is equipped with the Minkowski metric tensor already defined in the previous section.

On this base manifold one can define a set of linear coordinate functions $\{x^\mu\}$. In this coordinates Klein-Gordon equation assumes the form (2.55) or in a more compact form

$$(\square + m^2) \psi = 0, \quad (2.76)$$

where $\square = \frac{\partial^2}{\partial x_0^2} - \nabla^2$ is the d'Alembert operator.

This equation was proposed by Oskar Klein and Walter Gordon to describe relativistic electrons [48]. However, as electrons carry also a spin, the equation does not provide with a satisfactory description of them and it is suitable only for spinless particles. For instance it could describe composite particles like pions, or Higgs boson.

By associating a “symbol” to this differential operator by means of the functions $e^{\pm ip_\mu x^\mu}$, see Ref. [22], one can find a function on the cotangent bundle $T^*\mathbb{R}^4$ which is quadratical in the momentum four-vector of the relativistic particle

$$e^{\pm ip_\mu x^\mu} \square e^{\mp ip_\mu x^\mu} = p_\mu p^\mu. \quad (2.77)$$

The dispersion relation defined by means of the symbol above, determines a seven-dimensional submanifold Σ_m of the phase space $T^*\mathbb{R}^4$ as follows

$$\Sigma_m \equiv \{(x, p) \mid p^\mu p_\mu = m^2\}. \quad (2.78)$$

Denoting with i_Σ the canonical immersion of Σ_m into $T^*\mathbb{R}^4$, one has that the pull-back $i_\Sigma^*(\theta_0) = \theta_m$ of the natural Liouville one-form $\theta_0 = p_\mu dx^\mu$, defines a contact structure (see Appendix B for some basic definitions. A more detailed exposition can be found in [32]). Indeed a direct computation shows that:

$$\begin{aligned} \theta_m \wedge (d\theta_m)^3 &= (p^3 dp^0 \wedge dp^1 \wedge dp^2 - p^2 dp^0 \wedge dp^1 \wedge dp^3 + p^1 dp^0 \wedge dp^2 \wedge dp^3 + \\ &+ p^0 dp^1 \wedge dp^2 \wedge dp^3) \wedge dx^0 \wedge dx^1 \wedge dx^2 \wedge dx^3 \neq 0. \end{aligned}$$

As explained in the appendix, a contact structure is defined up to multiplication by a non vanishing function. Using as a reference one form the canonical Liouville one form, one can consider all the family obtained by means of a conformal factor. The adapted lifting of the Poincaré algebra from the configuration space to the phase space is obtained by requiring that the associated vector fields on the phase space preserve the chosen one form. The Lie algebra on which the lifted vector fields will close is the Poincaré algebra itself if the conformal factor is function of a Casimir. In particular, if the conformal factor is function of the Casimir $p^2 = p_\mu p^\mu$, then, on the submanifold Σ_m it becomes actually a constant. This means that the requirement of Poincaré invariance for the potential one-form on $T^*\mathbb{R}^4$ selects a particular contact form θ_m on Σ_m which is unique apart from a multiplicative constant.

It is worth noticing that both θ_0 and the submanifold $p^\mu p_\mu = m^2$ are manifestly Poincaré invariant.

Having obtained a contact structure out of the Klein-Gordon equation, let us now introduce the Jacobi bracket associated with it. As one can see from the definition (3.83) in appendix B, this bracket is entirely defined in terms of the exterior differential d and the contact one-form θ_m , hence, being these ingredients invariant with respect to the Poincaré group, the Jacobi bracket itself will be fully invariant with respect to Poincaré group.

As explained in appendix B, one may write the Jacobi bracket in terms of a suitable pair (Λ_Σ, Γ) . At this purpose, let us consider the following tensor fields on $T^*\mathbb{R}^4$

$$\Lambda_\Sigma = \left(g^{\mu\nu} - \frac{p^\mu p^\nu}{m^2} \right) \frac{\partial}{\partial p^\mu} \wedge \frac{\partial}{\partial x^\nu} \quad (2.79)$$

and

$$\Gamma = \frac{p^\mu}{m^2} \frac{\partial}{\partial x^\mu}. \quad (2.80)$$

It is easy to verify that even if we have used a set of coordinate functions of the full phase space, say (x^μ, p^μ) , these two tensors are actually written in terms of vector fields which are tangent to the submanifold Σ_m and therefore belong to the tensor fields built out of the tangent bundle of Σ_m . This follows because both of them vanish when contracted with the differential of the Casimir function.

Direct computations show that these two tensors satisfy all the properties discussed in appendix B. Therefore one can introduce the following bracket on the set of differentiable functions on Σ_m :

$$[f, g] = \Lambda_\Sigma(df, dg) + fL_\Gamma g - gL_\Gamma f. \quad (2.81)$$

According to this bracket, for instance, the four spacetime coordinate functions do not commute. At the quantum level they would not describe localization on space-time. Indeed one gets the following commutation relations

$$[x^\rho, x^\sigma] = \frac{x^\rho p^\sigma - x^\sigma p^\rho}{m^2} \quad (2.82)$$

$$[p^\rho, x^\sigma] = g^{\rho\sigma} \quad (2.83)$$

$$[p^\rho, p^\sigma] = 0. \quad (2.84)$$

Let us point out once more that both tensors fields Λ_Σ and Γ are invariant under the Poincaré group \mathcal{P} . Therefore the associated Lie algebra \mathfrak{p} acts as an algebra of derivations for the Jacobi bracket and maps the subalgebra of functions which are invariant under Γ into itself. Because \mathfrak{p} also preserves Λ_Σ it is also an algebra of derivations for the Poisson subalgebra associated with Λ_Σ and, consequently, when the bivector field is not degenerate it may be realized in terms of Hamiltonian vector fields associated with the conventional generators $M_\mu^\nu = x_\mu p^\nu - x_\nu p^\mu$ and p^μ .

The corresponding Hamiltonian vector fields in the sense of the Jacobi structure are the vector fields

$$X_{\rho\sigma} = q_\rho \frac{\partial}{\partial x^\sigma} - q_\sigma \frac{\partial}{\partial x^\rho} + p_\rho \frac{\partial}{\partial p^\sigma} - p_\sigma \frac{\partial}{\partial p^\rho} \quad (2.85)$$

$$X_\mu = \frac{\partial}{\partial x^\mu}, \quad (2.86)$$

and they coincide with the evaluation on the submanifold Σ_m of the generators of the canonical action of the Poincaré group on $T^*\mathbb{R}^4$ with respect to the symplectic structure $\omega = d\theta_0$.

It would be possible to realize this algebra also in terms of Hermitian operators, acting on square integrable functions on space-time. The physical interpretation of this realization, however, is not straightforward and it is connected with the definition of a time-operator in Quantum Mechanics, see [49].

Two final remarks before ending this digression. Firstly, this construction is quite general and could be dealt with in general abstract terms and for scalar operators not restricted to be second order. It would also be possible to consider Dirac-like operators by using the formulation in terms of Dirac-Kähler differential operators on differential forms (for more details see Ref. [50]).

Secondly, it is possible to introduce the same ingredients on the tangent bundle $T\mathbb{R}^4$. However the geometrical structure of the tangent bundle does not allow for the definition of a one form in a natural way and a Lagrangian

function is required in order to derive the analogue of the canonical Liouville one-form θ_0 . In particular, coming back to the covariant description of relativistic particles, one may consider on $T\mathbb{R}^4$ the Lagrangian

$$\mathcal{L} = \sqrt{g_{\mu\nu}v^\mu v^\nu},$$

where $g_{\mu\nu}$ is the Minkowski metric tensor. With this Lagrangian it is possible to associate the following one form [51, 41]

$$\theta_{\mathcal{L}} = \frac{\partial \mathcal{L}}{\partial x^\mu} dx^\mu = \frac{g_{\mu\nu}v^\nu}{\mathcal{L}} dx^\mu.$$

On the submanifold Σ , defined by the equation $g_{\mu\nu}v^\mu v^\nu = 1$, the pull-back of $\theta_{\mathcal{L}}$ to Σ defines a contact structure. The computations are analogous to the ones already presented in this paragraph: it is enough to replace p_μ with v_μ and fix $m^2 = 1$.

2.3.3 Beyond Peierls

After previous digressions, in this last paragraph we will adapt Peierls idea in order to get a Jacobi bracket. Once more the starting point is the definition of an action functional. Since we are interested in the description of test particles moving in a metric space, we will consider the following action functional:

$$S[\gamma] = \int_{s_0}^{s_1} \sqrt{g_{\mu\nu}v^\mu v^\nu} ds, \quad (2.87)$$

which describes geodesical motion of massive particles with mass $m = 1$.

Euler-Lagrange equations associated with the action functional (2.87) are

$$\frac{d}{ds} \left(\frac{g_{\mu\nu}\dot{x}^\nu}{\mathcal{L}} \right) = 0 \quad (2.88)$$

and a solution is a unparametrized geodesic, which for flat Minkowski space is given by an equivalence class of lines with constant velocities. For what is needed in the following part one can represent a solution by means of its momenta, which are

$$\frac{g_{\mu\nu}\dot{x}^\nu}{\mathcal{L}} = k_\mu.$$

Following Peierls one selects a reference solution γ_0 and linearize Euler-Lagrange equations around it. Considering the action functional (2.87) one obtains the following Jacobi operator acting on a variation $\delta\gamma$

$$\mathcal{J}_{\gamma_0}[\delta\gamma] = \frac{1}{\mathcal{L}} (g_{\mu\nu} - k_\mu k_\nu) \frac{d^2}{ds^2} \delta\gamma^\nu(s) = \frac{1}{\mathcal{L}} P_{\mu\nu} \frac{d^2}{ds^2} \delta\gamma^\nu(s). \quad (2.89)$$

Variations which are in the kernel of this operator (i.e. for variations which solve Jacobi equation) actually define the tangent space to any of the parametrized geodesic in the equivalence class of the solution γ_0 . As the scalar product

$$g_{\mu\nu}\delta\gamma^\mu\dot{\gamma}^\nu = \langle\delta\gamma, \dot{\gamma}\rangle \quad (2.90)$$

satisfies the equation

$$\frac{d^2}{ds^2} (\langle\delta\gamma, \dot{\gamma}\rangle) = 0, \quad (2.91)$$

it follows that $\langle\delta\gamma, \dot{\gamma}\rangle = as + b$ with a, b two constants. Therefore a solution of Jacobi equation for the variations can be always decomposed into the orthogonal sum:

$$J(s) = J_\perp(s) + (as + b)\dot{\gamma} \quad (2.92)$$

and $J_\perp(s)$ is such that $\langle J_\perp, \dot{\gamma}\rangle$ vanishes. Let us notice that this decomposition is possible only for time-like or space-like geodesics because in this case $\langle\dot{\gamma}, \dot{\gamma}\rangle = \text{const} \neq 0$. Light rays satisfy $\langle\dot{\gamma}, \dot{\gamma}\rangle = 0$ and the component J_\perp will have a non vanishing projection along $\dot{\gamma}$.

Let us fix now a given parametrization, for instance we will use proper time. This choice amounts to put $\langle\dot{\gamma}, \dot{\gamma}\rangle = 1$. Therefore solutions J of Jacobi equation which are compatible with this “gauge” choice satisfy the following condition

$$\left\langle \frac{d}{ds} J, \dot{\gamma} \right\rangle = \frac{d}{ds} \langle J, \dot{\gamma} \rangle = 0,$$

which implies that $\langle J, \dot{\gamma} \rangle$ is a conserved quantity along the geodesic. This allows to define the following one form on the space of geodesics:

$$\Theta(\gamma)[J] = \langle \dot{\gamma}, J \rangle \quad (2.93)$$

which defines a contact structure on the space of parametrized geodesics with $\langle\dot{\gamma}, \dot{\gamma}\rangle = 1$ [40]. In particular the component $J_\perp(s)$ are in the kernel of this one form, or in other words they are the contact elements relative to this contact structure.

Let us now consider the following difference:

$$J_1^\mu P_{\mu\nu} \frac{d^2}{ds^2} J_2^\nu - \frac{d^2}{ds^2} J_1^\mu P_{\mu\nu} J_2^\nu = \frac{d}{ds} \left(J_1^\mu P_{\mu\nu} \frac{d}{ds} J_2^\nu - \frac{d}{ds} J_1^\mu P_{\mu\nu} J_2^\nu \right). \quad (2.94)$$

The left hand side of this equation vanishes when evaluated on variations J^μ which are solution of Jacobi equation, which implies the conservation of the expression in round brackets on the right hand side. This conserved quantity defines a two form Ω on the space of geodesics and one immediately realizes that this two form is degenerate, the kernel being made of variations

$J(s) = (as + b)\dot{\gamma}(s)$. Therefore when one restricts this two form to a contact element we get a non degenerate antisymmetric bilinear operator.

A simple argument allows to show that this two-form is actually the differential of the one form Θ . Indeed if one fixes a given value of the parameter, for instance $s = 0$, each geodesic can be associated with its initial conditions $\{\gamma^\mu(s = 0), \frac{d}{ds}\gamma^\mu(s = 0)\} \equiv \{x^\mu, v^\mu\}$ and a solution $J(s)$ of the Jacobi equation with the initial conditions $\{J^\mu(s = 0), \frac{d}{ds}J^\mu(s = 0)\} \equiv \{\frac{\partial}{\partial x^\mu}, \frac{\partial}{\partial v^\mu}\}$. In these coordinates the one-form Θ is given by

$$\Theta = g_{\mu\nu}v^\mu dx^\nu,$$

whereas the two form Ω is written as

$$\Omega = P_{\mu\nu}dv^\mu \wedge dx^\nu = (g_{\mu\nu} - v_\mu v_\nu)dv^\mu \wedge dx^\nu.$$

Since $v_\mu dv^\mu = 0$ on the submanifold $v_\mu v^\mu = 1$, Ω coincide with the differential of Θ . Actually from this expression one can immediately notice the relationship with previous construction. The constraint that has been introduced in the previous paragraph can be seen as the constraint for the initial conditions of the solutions of a set of differential equations which come from a variational principle. Then the procedure outlined in this section permits to transport the geometrical structure of the initial conditions along the whole geodesic obtaining a description which does not require any splitting into space and time.

Up to now the contact structure has been defined. In order to write a Jacobi bracket we will adapt Peierls' idea to this setting. Indeed let us consider a functional $A[\gamma]$ defined on the space of geodesics. One can associate with this functional a function on the finite dimensional manifold of the initial conditions. However it is possible to avoid the splitting into space and time which is associated with the choice of a Cauchy surface and one can define a bivector field according to the procedure described in the previous sections. Therefore one can use the functional A to set a new variational principle where the new action functional is given by $S + \lambda A$. If one looks for solutions which are perturbations of a given solution γ_0 of the unmodified Euler-Lagrange equation, one gets the Jacobi equation with a source term, that is

$$\frac{1}{\mathcal{L}[\gamma_0]}P_{\mu\nu}[\gamma_0]\frac{d^2}{ds^2}\delta_A\gamma^\nu(s) = -\frac{\delta A}{\delta\gamma^\mu}. \quad (2.95)$$

Then we should select a solution $\tilde{\delta}\gamma_A^\nu(s)$ given in terms of the commutator Green function $\tilde{G}^{\mu\nu}(s - s')$ [43]

$$\tilde{\delta}\gamma_A^\nu(s) = \int_{\mathbb{R}} ds' \tilde{G}^{\nu\mu}(s - s') \frac{\delta A}{\delta\gamma^\mu}(s').$$

Since the Jacobi operator has a kernel it is not possible to invert the linearized equation. However one can look for a right inverse of this operator, i.e. one can look for fundamental solutions satisfying the following equation

$$\frac{1}{\mathcal{L}} P_{\mu\nu}[\gamma_0] \frac{d^2}{ds^2} G^{(\pm)\nu\rho}(s, s_0) = P_{\mu}^{\rho}[\gamma_0] \delta(s, s_0). \quad (2.96)$$

Eventually one gets the following commutator Green function

$$\tilde{G}^{\mu\nu}(s, s') = \mathcal{L} P^{\mu\nu}[\gamma_0](s - s'), \quad (2.97)$$

which is defined up to elements which are in the kernel of the Jacobi operator. When one restricts this operator to solutions that belong to a contact element it is no more degenerate and it coincides with the inverse of the two form Ω , for any possible choice of the right inverse $\tilde{G}^{\mu\nu}(s, s')$. Therefore this is a possible bivector Λ which can be used in the definition of a Jacobi bracket.

Let us now come back to the contact structure Θ . The corresponding Reeb field (see Appendix B) is given by the solution of the Jacobi equation $J(s) = \dot{\gamma}$ as can be proven by a direct computation:

$$\Theta(\gamma)[\dot{\gamma}] = \langle \dot{\gamma}, \dot{\gamma} \rangle = 1.$$

Eventually one can write a Jacobi bracket between two functionals A, B according to the following formula

$$\begin{aligned} [A, B](\gamma) &= \int_{\mathbb{R}} \int_{\mathbb{R}} ds ds' \frac{\delta A}{\delta \gamma^{\mu}}(s) \tilde{G}^{\mu\nu}(s - s') \frac{\delta B}{\delta \gamma^{\nu}}(s') + \\ &+ \int_{\mathbb{R}} \int_{\mathbb{R}} ds ds' A(s) \dot{\gamma}^{\mu}(s') \frac{\delta B}{\delta \gamma^{\mu}}(s') - \int_{\mathbb{R}} \int_{\mathbb{R}} ds ds' B(s) \dot{\gamma}^{\mu}(s) \frac{\delta A}{\delta \gamma^{\mu}}(s). \end{aligned} \quad (2.98)$$

This formula represents a generalization of the Peierls bracket in the form of a Jacobi bracket. The appearance of the vector field along the geodesics is reminiscent of the eleventh generator considered by Dirac [33]. A Poisson subalgebra is given by the set of functionals which are invariant under reparametrization of the geodesic, which are the functionals, say A , for which

$$\int_{\mathbb{R}} ds \dot{\gamma}^{\mu}(s) \frac{\delta A}{\delta \gamma^{\mu}}(s) = 0.$$

As an example one can compute the commutation relations between two functionals of the form

$$A = \int_{\mathbb{R}} x^{\mu} \delta(s - s_1) ds \quad B = \int_{\mathbb{R}} x^{\nu} \delta(s - s_2) ds$$

and the result is

$$[A, B](\gamma) = P^{\mu\nu}(s_1 - s_2) + x^\mu(s_1)k^\nu - x^\nu(s_2)k^\mu$$

For $s_1 = s_2$ one gets that

$$[A, B](\gamma) = x^\mu k^\nu - x^\nu k^\mu$$

which coincides with expression found in the previous paragraph, showing once more that space-time “positions” do not commute in this setting.

Chapter 3

Hamilton-Jacobi Approach to Potential Functions in Information Geometry

In this final chapter we will describe how it is possible to define a “canonical” potential function by means of a complete solution of a Hamilton-Jacobi equation which is associated with a suitable dynamical system [52].

Potential functions are a generalization of the divergence functions which have been introduced in information geometry in order to define the concept of relative entropy. Given a manifold with a metric tensor g and a symmetric tensor of order three T , a potential function is a two point function which contains all the information on this geometric structure. In particular by means of an algorithm it is possible to recover both tensors g and T and consequently a pair of dual connections which play a relevant role for instance in estimation theory (for an introduction to the methods of information geometry and the corresponding applications see [24, 25]).

After an introductory section in which we will shortly present some concepts of information geometry, the remaining part of this chapter will be devoted to the definition of the canonical potential function mentioned above. Then some aspect of such an approach will be further discussed.

3.1 An Introduction to Information Geometry

In this first section we will give a short introduction of the basic concepts of information geometry which will be used in the rest of the chapter. Among the pioneers of this approach to statistics there is Shun-Ichi Amari and the

most of the contents of this introduction comes from his book [24].

Information geometry began as the geometric study of statistical estimation. This study involves the interpretation of probability distributions over a measurable set as points of a manifold and consequently all the methods developed in differential geometry can be used to analyze statistical problems. Let us start with some definitions.

Let us consider a measurable set $(\chi, \mathcal{B})^1$, where χ is a set and \mathcal{B} is the algebra of all its measurable subsets [53]. A probability density is a function $p : \chi \rightarrow \mathbb{R}$ such that

$$p(x) \geq 0, \forall x \in \chi \quad (3.1)$$

$$\int_{\chi} p(x) d\mu = 1, \quad (3.2)$$

where $d\mu$ denotes the given measure on χ^2 .

The space of all probability densities can be equipped with the structure of a smooth infinite dimensional manifold (see [54]) called statistical manifold. However as far applications to estimation theory are concerned one can limit himself to the study of finite dimensional submanifolds, called statistical models. It is possible to build a statistical model by means of a smooth injective map which associates a probability density on χ with any point ξ of a manifold of parameters Ξ . An element of this model, therefore, will be a parametrized probability density $p_{\xi}(x)$, where $\xi \in \Xi$.

An example is the space of normal distributions where $\chi = \mathbb{R}$ and $\xi \equiv (\mu, \sigma) \in \Xi = \mathbb{R} \times \mathbb{R}_+$. A normal distribution is a probability density on \mathbb{R} parametrized as follows:

$$p_{(\mu, \sigma)}(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}. \quad (3.3)$$

This manifold can be equipped with a metric tensor g_F , called Fisher-Rao metric, which is invariant with respect to diffeomorphisms of χ . and plays a relevant role in inference problems (see [25] for a more recent review on the applications of information geometry). The components of g_F in a coordinate system $\{\xi^k\}$ are written as

$$g_{kl}(\xi) = E_{\xi}[\partial_k \log(p_{\xi}) \partial_l \log(p_{\xi})] = \int_{\chi} p(x) \partial_k \log(p_{\xi}(x)) \partial_l \log(p_{\xi}(x)) d\mu, \quad (3.4)$$

¹I will use the same symbol χ for both discrete and continuous sets. In case of a finite set the symbol \int has the meaning of a sum over the points of the set.

²In a more general treatment one should consider probability measure dp absolutely continuous with respect to the given measure $d\mu$. Consequently the probability density $p(x)$ is the Radon-Nikodym derivative of the measure dp with respect to $d\mu$.

where $E_\xi[\cdot]$ denotes the expectation value with respect to the probability distribution associated with the point $\xi \in \Xi$.

Remark 8 *More generally Fisher-Rao metric is invariant with respect to a wider class of transformation called sufficient statistics (see [24]). This theorem was proven by Cencov in [55] in the case of finite measure spaces χ and extended to the space of all probability densities on a compact manifold with boundary in [54].*

Another tensor of interest for the applications of information geometry to inference problems is a symmetric tensor T of order three, called skewness tensor, which in coordinate has the following components

$$T_{jkl}(\xi) = E_\xi[\partial_j \log(p_\xi) \partial_k \log(p_\xi) \partial_l \log(p_\xi)]. \quad (3.5)$$

By means of this symmetric tensor is possible to build a family of dual torsion-less connections called α -connections. A pair (∇, ∇^*) defines a pair of dual connections with respect to a metric tensor g iff the following equality is satisfied:

$$L_X (g(Y, Z)) = (g(\nabla_X Y, Z)) + (g(Y, \nabla_X^* Z)) , \quad (3.6)$$

for any vector field X, Y, Z . Here L_X denotes the Lie derivative with respect to the vector field X and ∇_X is the covariant derivative with respect to the vector field X associated with the connection ∇ . According to this definition the only self-dual torsionless connection is the Levi-Civita connection.

The Christoffel symbols of a α -connection can be written as follows:

$$\Gamma_{jkl}^{(\alpha)} = \Gamma_{jkl}^{(0)} - \frac{\alpha}{2} T_{jkl} , \quad (3.7)$$

where $\Gamma_{jkl}^{(0)}$ are the Christoffel symbols of the Levi-Civita connection associated with the Fisher-Rao metric (3.4). The pair of connections $(\nabla^{(\alpha)}, \nabla^{(-\alpha)})$ forms a pair of dual connections with respect to Fisher-Rao metric.

From a more abstract point of view it is possible to define a statistical model as a triple (Ξ, g, T) where Ξ is a manifold the points of which parametrize a family of probability densities, g is a metric tensor and T is a symmetric tensor of order three.

It is possible to prove (see for instance [56, 24]) that the geometrical structure of every statistical model can be completely encoded in a two-point function $S: \Xi \times \Xi \rightarrow \mathbb{R}$ called contrast function. This is a distance-like function such that:

$$S(\xi_1, \xi_2) \geq 0 \quad \forall (\xi_1, \xi_2) \in \Xi \times \Xi, \quad (3.8)$$

$$S(\xi_1, \xi_2) = 0 \quad \text{iff } \xi_1 = \xi_2. \quad (3.9)$$

Here, the first Ξ is thought of as the manifold of initial points whose coordinates are denoted by q_{in} , and the second Ξ is the manifold of final points whose coordinates are denoted by q_{fin} . If S is at least C^3 it follows that (see [56] for more details):

$$\left. \frac{\partial S}{\partial q_{\text{in}}^j} \right|_{q_{\text{in}}=q_{\text{fin}}} = \left. \frac{\partial S}{\partial q_{\text{fin}}^j} \right|_{q_{\text{in}}=q_{\text{fin}}} = 0. \quad (3.10)$$

The metric g and the tensor T are recovered from it as follows:

$$\left. \frac{\partial^2 S}{\partial q_{\text{in}}^j \partial q_{\text{in}}^k} \right|_{q_{\text{in}}=q_{\text{fin}}} = \left. \frac{\partial^2 S}{\partial q_{\text{fin}}^j \partial q_{\text{fin}}^k} \right|_{q_{\text{in}}=q_{\text{fin}}} = - \left. \frac{\partial^2 S}{\partial q_{\text{fin}}^j \partial q_{\text{in}}^k} \right|_{q_{\text{in}}=q_{\text{fin}}} = g_{jk}, \quad (3.11)$$

$$\left. \frac{\partial^3 S}{\partial q_{\text{in}}^l \partial q_{\text{fin}}^k \partial q_{\text{fin}}^j} \right|_{q_{\text{in}}=q_{\text{fin}}} - \left. \frac{\partial^3 S}{\partial q_{\text{fin}}^l \partial q_{\text{in}}^k \partial q_{\text{in}}^j} \right|_{q_{\text{in}}=q_{\text{fin}}} = T_{jkl}. \quad (3.12)$$

It is important to note that S is never unique, and this leads to the need for the definition of a contrast function which is canonical in some suitable sense [57].

3.2 A Canonical Potential Function

After introducing some necessary vocabulary we will present in this section a recent proposal [52] by Ciaglia et al. They suggest to interpret the task of finding a canonical potential function for the statistical model (Ξ, g, T) in the context of Hamilton-Jacobi theory associated with a particular Lagrangian built directly from the metric g and the symmetric tensor T . Note that the dynamical approach to potential functions presented here is purely geometric in the sense that it relies only on the geometrical structure of Ξ . This means that Ξ needs not to be a statistical manifold endowed with the Fisher-Rao metric and the canonical skewness tensor of information geometry, but it could be a generic manifold endowed with a generic metric tensor g and a generic skewness tensor T . This is particularly useful with respect to quantum mechanics, where quantum states are probability amplitudes and not genuine probability distributions, and where, for invertible mixed states,

there is an infinite number of possible generalizations of the Fisher-Rao metric³ ([58], [59]).

The fact that S is a two-point function allows to read the problem of finding a canonical contrast function on a statistical manifold as the Hamilton-Jacobi problem associated with suitable Lagrangian and Hamiltonian functions. Indeed, let us consider a statistical model (Ξ, g, T) , let $\alpha \neq 0$ be a real number, and let us define the following Lagrangian function

$$\mathfrak{L}_\alpha(q, v) = \frac{1}{2}g_{jk}(q)v^jv^k + \frac{\alpha}{6}T_{jkl}(q)v^jv^kv^l. \quad (3.13)$$

A complete solution S_α of the Hamilton-Jacobi equation associated with this Lagrangian is a potential function for our statistical model in the sense that it allows to recover the geometric structure of the manifold as follows:

$$\left. \frac{\partial^2 S_\alpha}{\partial q_{\text{fin}}^j \partial q_{\text{in}}^k} \right|_{q_{\text{in}}=q_{\text{fin}}} = -g_{jk}, \quad (3.14)$$

$$\left. \frac{\partial^3 S_\alpha}{\partial q_{\text{in}}^l \partial q_{\text{in}}^k \partial q_{\text{fin}}^j} \right|_{q_{\text{in}}=q_{\text{fin}}} - \left. \frac{\partial^3 S_\alpha}{\partial q_{\text{fin}}^l \partial q_{\text{fin}}^k \partial q_{\text{in}}^j} \right|_{q_{\text{in}}=q_{\text{fin}}} = 2\alpha T_{jkl}. \quad (3.15)$$

Equation (3.15) is slightly different from equation (3.12), consequently, the name potential function has been chosen instead of contrast function for S_α because S_α allows to recover the geometrical structures of the statistical manifold. Notice further that S_α does not need to be positive semidefinite, while a contrast function must be so.

Remark 9 *In the following, the term “contrast function” will be used for a two-point function satisfying the conditions given in equations (3.8) and (3.9). The term “potential function” will be employed for a generic two-point function by means of which it is possible to recover the geometrical structure of a statistical manifold (Ξ, g, T) using a suitably defined procedure, such as that given by equations (3.14) and (3.15).*

Note that it is possible to write the Lagrangian (3.13) in intrinsic form as follows:

$$\mathfrak{L}_\alpha = \mathfrak{L}_g + \frac{1}{3}L_{\alpha\Gamma}\mathfrak{L}_g, \quad (3.16)$$

³These are metric tensors satisfying the so-called monotonicity property, i.e., the scalar product they induce on tangent vectors does not increase under the action of completely positive trace-preserving (CPTP) maps.

where \mathfrak{L}_g is the metric Lagrangian associated with g and ${}_\alpha\Gamma$ is the second order vector field [41] associated to the affine connection ∇^α (3.7). By looking at this expression one can notice that this Lagrangian can be considered as a sort of first-order approximation of a more complete function $\widetilde{\mathfrak{L}}_\alpha$ which also includes all successive Lie derivatives with respect to the vector field Γ , shortly:

$$\widetilde{\mathfrak{L}}_\alpha = e^{\tau L_{\alpha\Gamma}} \mathfrak{L}_g = (\Phi_\tau^\alpha)^* \mathfrak{L}_g, \quad (3.17)$$

where Φ_τ^α is the flow of the second order vector field ${}_\alpha\Gamma$ on the tangent bundle $T\Xi$ of the statistical manifold Ξ . However, only (3.16) contributes to the determination of metric and skewness tensors, as it will be proven in the following.

Since S_α is the generating function of a canonical transformation, the following relations are valid:

$$p_j^{\text{in}} = -\frac{\partial S_\alpha}{\partial q_{\text{in}}^j}, \quad (3.18)$$

$$p_j^{\text{fin}} = \frac{\partial S_\alpha}{\partial q_{\text{fin}}^j}, \quad (3.19)$$

where $\{p_j^{\text{in}}\}$ (resp. $\{p_j^{\text{fin}}\}$) are the canonical momenta associated to q_{in}^j 's (resp. q_{fin}^j 's).

Furthermore, the momenta p_j can be expressed in terms of the Lagrangian function as:

$$p_j = \frac{\partial \mathfrak{L}}{\partial v^j}, \quad (3.20)$$

in particular, for the Lagrangian under investigation one gets:

$$p_j = g_{jk}(q)v^k + \frac{\alpha}{2} T_{jkl}(q)v^k v^l. \quad (3.21)$$

From this, it follows that:

$$\frac{\partial S_\alpha}{\partial q_{\text{in}}^j} = -p_j^{\text{in}} = -g_{jk}(q_{\text{in}})v_{\text{in}}^k - \frac{\alpha}{2} T_{jkl}(q_{\text{in}})v_{\text{in}}^k v_{\text{in}}^l, \quad (3.22)$$

where the v_{in}^j 's must be expressed in terms of the initial and final positions. The link between initial and final positions ($q_{\text{in}}, q_{\text{fin}}$) and the initial velocity (v_{in}) is provided by the dynamical trajectories γ_c associated with the Lagrangian \mathfrak{L} . The Euler-Lagrange equations associated with \mathfrak{L} are:

$$\begin{aligned} (g_{jk}(q) + \alpha T_{jkl} v^l) \dot{v}^k &= -{}_g \Gamma_{jkl} v^l v^k + \\ & - \frac{\alpha}{6} \left(\frac{\partial T_{jkl}}{\partial q^m} + \frac{\partial T_{jlm}}{\partial q^k} + \frac{\partial T_{jkm}}{\partial q^l} - \frac{\partial T_{klm}}{\partial q^j} \right) v^k v^l v^m, \end{aligned} \quad (3.23)$$

where $v^j = \frac{dq^j}{dt}$ and $\dot{v}^j = \frac{dv^j}{dt}$. A series expansion of $\gamma_c(t) = (q^1(t), \dots, q^n(t))$ around $t = 0$ yields:

$$q^j(t) = q_{\text{in}}^j + t \left. \frac{dq^j}{dt} \right|_{t=0} + \frac{t^2}{2} \left. \frac{d^2 q^j}{dt^2} \right|_{t=0} + \mathcal{O}(t^3). \quad (3.24)$$

One knows that $v_{\text{in}} = \left. \frac{dq^j}{dt} \right|_{t=0}$, so that naming $q_{\text{fin}}^j := q^j(1)$, it is possible to write:

$$v_{\text{in}}^j = q_{\text{fin}}^j - q_{\text{in}}^j - \frac{1}{2} \left. \frac{dv_{\text{in}}^j}{dt} \right|_{t=0}, \quad (3.25)$$

where higher order terms in the expansion have been neglected. Since v_{in} is function of $q_{\text{in}}, q_{\text{fin}}$, one can express the derivatives with respect to q_{fin} in terms of the derivatives of v_{in} and viceversa. Indeed⁴:

$$\frac{\partial}{\partial q_{\text{fin}}^j} = \frac{\partial v_{\text{in}}^k}{\partial q_{\text{fin}}^j} \frac{\partial}{\partial v_{\text{in}}^k}, \quad (3.26)$$

$$\frac{\partial^2}{\partial q_{\text{fin}}^k \partial q_{\text{fin}}^j} = \frac{\partial^2 v_{\text{in}}^l}{\partial q_{\text{fin}}^k \partial q_{\text{fin}}^j} \frac{\partial}{\partial v_{\text{in}}^l} + \frac{\partial v_{\text{in}}^l}{\partial q_{\text{fin}}^j} \frac{\partial v_{\text{in}}^r}{\partial q_{\text{fin}}^k} \frac{\partial}{\partial v_{\text{in}}^r} \frac{\partial}{\partial v_{\text{in}}^l}, \quad (3.27)$$

and all these expressions need to be evaluated on the diagonal $q_{\text{fin}} = q_{\text{in}}$. Note that the condition $q_{\text{fin}} = q_{\text{in}}$ is equivalent to the fact that the dynamical trajectory is $q^j(t) = q_{\text{in}}^j$, and thus, according to the equations of motion, this corresponds to $v_{\text{in}} = 0$.

Equation (3.23) can be written as follows:

$$\dot{v}^l = -\alpha T_{jk}^l v^k \dot{v}^j - {}_g \Gamma_{kj}^l v^j v^k - \frac{\alpha}{6} g^{lj} \left(\frac{\partial T_{jkr}}{\partial q^m} + \frac{\partial T_{jrm}}{\partial q^k} + \frac{\partial T_{jkm}}{\partial q^r} - \frac{\partial T_{krm}}{\partial q^j} \right) v^k v^r v^m. \quad (3.28)$$

If one supposes that \dot{v}^j is an analytic function of $\{v^j\}$ in a neighbourhood of $v^j = 0$, it is possible to write:

⁴Note that, at this level, formula (3.26) and (3.27) are valid for every dynamical curve γ .

$$\dot{v}^k = \sum_{m=0}^{\infty} \sum_{j_1, \dots, j_m=1}^n a_{j_1 \dots j_m}^k v^{j_1} \dots v^{j_m}. \quad (3.29)$$

By inserting this expression into equation (3.23) one gets the coefficients

$$a_0^k = 0, \quad (3.30)$$

$$a_{j_1}^k = 0, \quad (3.31)$$

$$a_{j_1 j_2}^k = -g \Gamma_{j_1 j_2}^k, \quad (3.32)$$

and so on.

Therefore \dot{v}^j is a function of order $\mathcal{O}(|v|^2)$ and higher order derivatives $\{\ddot{v}^j, \dots\}$ will be at least of order $\mathcal{O}(|v|^3)$. These results can be put into equation (3.25) to obtain

$$v_{\text{in}}^j = q_{\text{fin}}^j - q_{\text{in}}^j + \frac{1}{2} g \Gamma_{kl}^j v_{\text{in}}^k v_{\text{in}}^l + \mathcal{O}(|v|^3). \quad (3.33)$$

Deriving this expression with respect to q_{fin} and then evaluating it at $v_i = 0$ one has

$$\left. \frac{\partial v_i^k}{\partial q_{\text{fin}}^j} \right|_{q_{\text{in}}=q_{\text{fin}}} = \delta_j^k, \quad (3.34)$$

$$\left. \frac{\partial^2 v_i^l}{\partial q_{\text{fin}}^k \partial q_{\text{fin}}^j} \right|_{q_{\text{in}}=q_{\text{fin}}} = g \Gamma_{jk}^l. \quad (3.35)$$

Eventually one has:

$$\left. \frac{\partial^2 S_\alpha}{\partial q_{\text{fin}}^k \partial q_{\text{in}}^j} \right|_{q_{\text{in}}=q_{\text{fin}}} = - \left. \frac{\partial p_j^{\text{in}}}{\partial v_{\text{in}}^k} \right|_{v_{\text{in}}=0} = -g_{jk}, \quad (3.36)$$

$$\left. \frac{\partial^3 S_\alpha}{\partial q_{\text{fin}}^l \partial q_{\text{fin}}^k \partial q_{\text{in}}^j} \right|_{q_{\text{in}}=q_{\text{fin}}} = -g \Gamma_{kl}^r \left. \frac{\partial p_j^{\text{in}}}{\partial v_{\text{in}}^r} \right|_{v_{\text{in}}=0} - \left. \frac{\partial^2 p_j^{\text{in}}}{\partial v_{\text{in}}^l \partial v_{\text{in}}^k} \right|_{v_{\text{in}}=0} = -g \Gamma_{jkl} - \alpha T_{jkl}. \quad (3.37)$$

From them it follows immediately that the metric tensor is derived from the metric Lagrangian only, whereas information about the connection depends on the “interaction term”, as it should be since quadratic terms alone cannot contribute to third order derivatives. In particular, when $\alpha = 0$ the

Christoffel symbols of the Levi-Civita connection associated to the metric g are obtained.

In order to extract the symmetric tensor from the potential function S_α it is necessary to take derivatives in a different order, according to equation (3.15). The main difference with respect to the previous description is the fact that

$$\frac{\partial S_\alpha}{\partial q_{\text{fin}}^j} = p_j^{\text{fin}}, \quad (3.38)$$

which is the canonical momentum at the extreme $\gamma(t=1) = q_{\text{fin}}$.

Following the procedure just outlined, one has to express the dependence of v_{fin} on the variables $(q_{\text{in}}, q_{\text{fin}})$. This relation is provided by the dynamics, which is reversible. Then it follows that

$$v_{\text{fin}}^j = q_{\text{fin}}^j - q_{\text{in}}^j - \frac{1}{2} g \Gamma_{kl}^j v_{\text{fin}}^k v_{\text{fin}}^l + \mathcal{O}(|v|^3). \quad (3.39)$$

Eventually the following result is valid:

$$\left. \frac{\partial^2 S_\alpha}{\partial q_{\text{in}}^k \partial q_{\text{fin}}^j} \right|_{q_{\text{in}}=q_{\text{fin}}} = - \left. \frac{\partial p_j^{\text{fin}}}{\partial v_{\text{fin}}^k} \right|_{v_{\text{fin}}=0} = -g_{jk}, \quad (3.40)$$

$$\left. \frac{\partial^3 S_\alpha}{\partial q_{\text{in}}^l \partial q_{\text{in}}^k \partial q_{\text{fin}}^j} \right|_{q_{\text{in}}=q_{\text{fin}}} = - \left. g \Gamma_{kl}^r \frac{\partial p_j^{\text{fin}}}{\partial v_{\text{fin}}^r} \right|_{v_{\text{fin}}=0} + \left. \frac{\partial^2 p_j^{\text{fin}}}{\partial v_{\text{fin}}^l \partial v_{\text{fin}}^k} \right|_{v_{\text{fin}}=0} = -g \Gamma_{jkl} + \alpha T_{jkl}. \quad (3.41)$$

From equations (3.14) and (3.15) it follows that S_α is actually a potential function for the statistical model (Ξ, g, T) . Note that S_α needs not to be positive as a contrast function would be, however this is not an obstruction in determining metric and skewness tensors. Indeed it is sufficient that S_α has a local extreme on the diagonal $q_{\text{in}} = q_{\text{fin}}$ (or $v = 0$), and it is true in this case as shown above, by calculating the Hessian matrices (3.36), (3.40). Furthermore, as already noticed, one could also think to add other interaction terms to the basic Lagrangian (3.16), and by a suitable choice of the coupling constants it is possible to make the contrast function positive definite.

3.3 Some Comments

This section will be dedicated to the discussion of some aspects related to this approach for defining canonical potential functions.

Let us start pointing out the connection between the potential function S_α defined here and the canonical contrast function defined on self-dual statistical model ([24]). A self-dual manifold is a statistical model for which the symmetric tensor T identically vanishes, so that the associated connection is the self-dual Levi-Civita connection ∇_g associated with the metric g .

For self-dual manifolds, a canonical contrast function S_d exists which is given by:

$$S_d(\mathbf{q}_{\text{in}}, \mathbf{q}_{\text{fin}}) = \frac{1}{2} d^2(\mathbf{q}_{\text{in}}, \mathbf{q}_{\text{fin}}), \quad (3.42)$$

where $d^2(q_{\text{in}}, q_{\text{fin}})$ is the square of the Riemannian geodesic distance associated with the metric g on \mathcal{M} .

Applying the procedure outlined in previous section to the case of self-dual manifolds, it is clear that the derived potential function is precisely the canonical contrast function S_d defined above. To see this, recall that the metric Lagrangian \mathfrak{L}_g associated with the metric tensor g , and all of its functions $F(\mathfrak{L}_g)$ with F analytic, give rise to the same dynamical trajectories ([41]). Furthermore, \mathfrak{L}_g and $F(\mathfrak{L}_g)$ are all constants of the motion for the dynamics. Denoting with γ_c the geodesic connecting $\mathbf{q}_{\text{in}} = \gamma_c(0)$ and $\mathbf{q}_{\text{fin}} = \gamma_c(1)$, this implies that:

$$I_{F(\mathfrak{L}_g)}(\mathbf{q}_{\text{in}}, \mathbf{q}_{\text{fin}}) := \int_{t_{\text{in}}}^{t_{\text{fin}}} F(\mathfrak{L}_g) dt = F(\mathfrak{L}_g)|_{\gamma_c(t)}. \quad (3.43)$$

Now, the Riemannian geodesic distance $d(q_{\text{in}}, q_{\text{fin}})$ is given by:

$$d(\mathbf{q}_{\text{in}}, \mathbf{q}_{\text{fin}}) = \int_{t_{\text{in}}}^{t_{\text{fin}}} \sqrt{2\mathfrak{L}_g} dt, \quad (3.44)$$

and thus:

$$\begin{aligned} d^2(\mathbf{q}_{\text{in}}, \mathbf{q}_{\text{fin}}) &= \left(\int_{t_{\text{in}}}^{t_{\text{fin}}} \sqrt{2\mathfrak{L}_g} dt \right)^2 = \left(\sqrt{2\mathfrak{L}_g} \right)^2 \Big|_{\gamma_c(t)} = \\ &= 2\mathfrak{L}_g|_{\gamma_c(t)} = 2 \int_{t_{\text{in}}}^{t_{\text{fin}}} \mathfrak{L}_g dt = 2 I_{\mathfrak{L}_g}(\mathbf{q}_{\text{in}}, \mathbf{q}_{\text{fin}}) \end{aligned} \quad (3.45)$$

It is immediate to realize that the Hamilton characteristic function associated with the Lagrangian $\mathfrak{L}_\alpha = \mathfrak{L}_g$ is precisely the canonical contrast function of equation (3.42).

A physically interesting example of self-dual manifold is given by the manifold $\mathcal{P}(\mathcal{H})$ of pure states of quantum mechanics. As it is shown in [60],

a meaningful notion of statistical distance between pure states can be defined by means of the concepts of distinguishability and statistical fluctuations in the outcomes of measurements. It turns out that this two-point function on pure states coincides with the Riemannian geodesic distance associated with the Fubini-Study metric, so that the statistical structure determined by this two-point function makes $\mathcal{P}(\mathcal{H})$ a self-dual manifold. Consequently, we can apply our procedure and conclude that the statistical distance introduced by Wotters coincides with the Hamilton principal function associated with the metric Lagrangian of the Fubini-Study metric on $\mathcal{P}(\mathcal{H})$. The relevance of the statistical structure on $\mathcal{P}(\mathcal{H})$ emerging from Wotter's statistical distance is enforced by the results of [61, 62], where it is shown that the set of pure states of quantum mechanics does not admit a dually flat statistical structure.

Now, consider the statistical model (Ξ, g, T) , where $\Xi = \mathbb{R}^+$, $g = \frac{1}{\xi^2}$, ${}^g\Gamma = -\frac{1}{\xi}$ is the Christoffel symbol of the Levi-Civita connection and $T = -\frac{2}{\xi^3}$. This manifold arises as the statistical model associated to the exponential distributions

$$p(x, \xi) = \xi e^{-x\xi} \quad \xi, x > 0. \quad (3.46)$$

The metric g and the tensor T are then obtained by:

$$g = \int_0^{+\infty} p(x, \xi) \left(\frac{d \log(p)}{d\xi} \right)^2 dx, \quad (3.47)$$

$$T = \int_0^{+\infty} p(x, \xi) \left(\frac{d \log(p)}{d\xi} \right)^3 dx. \quad (3.48)$$

The ‘‘deformed’’ Lagrangian function \mathfrak{L} with respect to the connection ∇ reads:

$$\mathfrak{L}_\alpha = \frac{v^2}{2\xi^2} - \frac{\alpha v^3}{3\xi^3}, \quad (3.49)$$

where $\mathfrak{L}_g = \frac{v^2}{2\xi^2}$ is the metric Lagrangian. It is clear that \mathfrak{L}_α is a function of \mathfrak{L}_g , specifically, it is $\mathfrak{L}_\alpha = \mathfrak{L}_g + \frac{2\sqrt{2}\alpha}{3} (\mathfrak{L}_g)^{\frac{3}{2}}$. Consequently, the solutions of the Euler-Lagrange equations associated with the metric Lagrangian \mathfrak{L}_g , i.e., the geodesics of g , are solutions of the Euler-Lagrange equations associated with the Lagrangian \mathfrak{L}_α , and the explicit expression of the dynamical trajectories $\gamma_c(t) = \xi(t)$ is:

$$\xi(t) = \xi_{\text{in}} e^{\frac{v_{\text{in}}}{\xi_{\text{in}}} t}. \quad (3.50)$$

A complete solution of the Hamilton-Jacobi problem for \mathfrak{L} is given by:

$$I_\alpha(\gamma_c) = \int_{t_{\text{in}}}^{t_{\text{fin}}} \mathfrak{L}_\alpha(\gamma_c(t), \dot{\gamma}_c(t)) dt, \quad (3.51)$$

where the curve γ_c has fixed extreme points $\xi_{\text{in}} = \gamma_c(t_{\text{in}})$ and $\xi_{\text{fin}} = \gamma_c(t_{\text{fin}})$, and integration is performed between $t_{\text{in}} = 0$ and $t_{\text{fin}} = 1$. In this case, since the Lagrangian \mathfrak{L}_α is a constant of the motion, one gets:

$$I_\alpha(\gamma_c) = \frac{v_{\text{in}}^2}{2\xi_{\text{in}}^2} - \frac{\alpha v_{\text{in}}^3}{3\xi_{\text{in}}^3}. \quad (3.52)$$

The link between $\xi_{\text{fin}}, \xi_{\text{in}}$ and v_{in} can easily be extracted from the explicit expression of $\gamma_c(t)$, indeed:

$$v_{\text{in}} = \xi_{\text{in}} \ln \left(\frac{\xi_{\text{fin}}}{\xi_{\text{in}}} \right), \quad (3.53)$$

and thus, the contrast function S reads:

$$S_\alpha(\xi_{\text{in}}, \xi_{\text{fin}}) = \frac{\ln^2 \left(\frac{\xi_{\text{fin}}}{\xi_{\text{in}}} \right)}{2} - \frac{\alpha}{3} \ln^3 \left(\frac{\xi_{\text{fin}}}{\xi_{\text{in}}} \right). \quad (3.54)$$

An explicit calculation gives:

$$\left. \frac{\partial^2 S_\alpha}{\partial \xi_{\text{fin}} \partial \xi_{\text{in}}} \right|_{\xi_{\text{in}} = \xi_{\text{fin}} = \xi} = -\frac{1}{\xi^2}, \quad (3.55)$$

$$\left. \frac{\partial^3 S_\alpha}{\partial \xi_{\text{fin}} \partial \xi_{\text{fin}} \partial \xi_{\text{in}}} \right|_{\xi_{\text{fin}} = \xi_{\text{in}} = \xi} = \frac{2\alpha + 1}{\xi^3} = -{}_g\Gamma - \alpha T, \quad (3.56)$$

$$\left. \frac{\partial^3 S_\alpha}{\partial \xi_{\text{fin}} \partial \xi_{\text{in}} \partial \xi_{\text{in}}} \right|_{\xi_{\text{fin}} = \xi_{\text{in}} = \xi} = \frac{1 - 2\alpha}{\xi^3} = -{}_g\Gamma + \alpha T, \quad (3.57)$$

showing that S_α is a potential function for the statistical model (Ξ, g, T) of exponential distributions.

The statistical structure of Ξ can be alternatively derived starting with the Kullback-Leibler divergence function S_{KL} :

$$S_{KL}(\xi_{\text{in}}, \xi_{\text{fin}}) = \int_0^{+\infty} p(x, \xi_{\text{in}}) \ln \left(\frac{p(x, \xi_{\text{in}})}{p(x, \xi_{\text{fin}})} \right) dx = \ln \left(\frac{\xi_{\text{in}}}{\xi_{\text{fin}}} \right) + \frac{\xi_{\text{fin}}}{\xi_{\text{in}}} - 1. \quad (3.58)$$

Kullback-Leibler divergence function plays an important role in information theory since it defines the mutual information of two probability distribution. As it is clear, the potential function S_α in equation (3.54) does not coincide with the Kullback-Leibler divergence. This is not surprising since, for a given statistical model, there are infinitely many potential (contrast) functions generating the same statistical structure. However, it is possible to read the Kullback-Leibler divergence S_{KL} as the Hamilton principal function I_{KL} associated with a suitably defined Lagrangian. At this purpose, let us perform the following diffeomorphism between $\Xi = \mathbb{R}_+$ and $\Theta = \mathbb{R}$:

$$\xi \mapsto y = \ln(\xi). \quad (3.59)$$

This diffeomorphism gives rise to a diffeomorphism between $\Xi \times \Xi$ and $\Theta \times \Theta$:

$$(\xi_{\text{in}}, \xi_{\text{fin}}) \mapsto (y_{\text{in}} = \ln(\xi_{\text{in}}), y_{\text{fin}} = \ln(\xi_{\text{fin}})). \quad (3.60)$$

The Kullback-Leibler divergence S_{KL} becomes:

$$S_{KL}(y_{\text{in}}, y_{\text{fin}}) = e^{(y_{\text{fin}} - y_{\text{in}})} - (y_{\text{fin}} - y_{\text{in}}) - 1. \quad (3.61)$$

Now, consider the following Lagrangian on $T\Theta$:

$$\mathfrak{L}_{KL}(y, u) = e^u - u - 1, \quad (3.62)$$

and let us calculate the Hamilton principal function associated with \mathfrak{L}_{KL} . Since \mathfrak{L}_{KL} depends only on the velocity coordinate u , it is an alternative Lagrangian for the 1-dimensional free-particle on $\mathcal{N} = \mathbb{R}$ ([41]). Consequently, the dynamical trajectories of the system coincide with the geodesics of the Euclidean metric, that is, they are straight lines $\gamma_c(t) = v_{\text{in}}t + y_{\text{in}}$. Setting $t_{\text{in}} = 0, t_{\text{fin}} = 1$, the connection between $y_{\text{in}}, y_{\text{fin}}$ and v_{in} is easily seen to be $v_{\text{in}} = y_{\text{fin}} - y_{\text{in}}$. Furthermore, \mathfrak{L}_{KL} is a constant of the motion, and thus, it can be brought out from the integral defining the Hamilton principal function:

$$I_{KL}(y_{\text{in}}, y_{\text{fin}}) = \mathfrak{L}_{KL}(y_{\text{in}}, v_{\text{in}}(y_{\text{in}}, y_{\text{fin}})) = e^{(y_{\text{fin}} - y_{\text{in}})} - (y_{\text{fin}} - y_{\text{in}}) - 1. \quad (3.63)$$

Confronting equations (3.61) and (3.63), one can conclude that the Hamilton principal function associated with \mathfrak{L}_{KL} is precisely the Kullback-Leibler divergence S_{KL} as claimed.

Let us point out now an interesting connection between the Lagrangian \mathfrak{L}_{KL} associated with the Kullback-Leibler divergence of equation (3.58) and the Lagrangian \mathfrak{L}_α associated with the potential function of equation (3.54). At this purpose, let us apply the tangent lift of the diffeomorphism given by equation (3.59) to the Lagrangian \mathfrak{L}_α of equation (3.49):

$$\mathfrak{L}_\alpha(y, u) = \frac{u^2}{2} - \frac{\alpha}{3} u^3. \quad (3.64)$$

Now, let us perform a series expansion of \mathfrak{L}_{KL} around $u = 0$:

$$\mathfrak{L}_{KL}(y, u) = \frac{u^2}{2} + \frac{u^3}{6} + \mathcal{O}(u^4). \quad (3.65)$$

Confronting equations (3.64) and (3.65) one immediately sees that, upon taking $\alpha = -\frac{1}{2}$, the Lagrangian \mathfrak{L}_α is precisely the third order approximation of \mathfrak{L}_{KL} .

This line of reasoning can be pushed a little further, and show that, if the Kullback-Leibler divergence S_{KL} generating the statistical structure of a statistical manifold (Ξ, g, T) is the Hamilton principal function associated with a Lagrangian \mathfrak{L}_{KL} , then the Lagrangian \mathfrak{L}_α proposed here is the third order approximation of \mathfrak{L}_{KL} up to a constant factor, and provided one choose $\alpha = -\frac{1}{2}$.

Let us consider a statistical model (Ξ, g, T) and the Kullback-Leibler divergence S_{KL} generating the statistical structure of Ξ . Let us assume that S_{KL} admits a Lagrangian \mathfrak{L}_{KL} such that S_{KL} is the Hamilton principal function associated with \mathfrak{L}_{KL} . Assuming \mathfrak{L}_{KL} analytic in \mathbf{v} as in the previous section, an expansion of \mathfrak{L}_{KL} in a power series of the velocity vector \mathbf{v} around $\mathbf{v} = 0$ gives:

$$\begin{aligned} \mathfrak{L}_{KL} = & \mathfrak{L}_{KL}|_{\mathbf{v}=0} + \left. \frac{\partial \mathfrak{L}_{KL}}{\partial v^j} \right|_{\mathbf{v}=0} v^j + \left. \frac{\partial^2 \mathfrak{L}_{KL}}{\partial v^j \partial v^k} \right|_{\mathbf{v}=0} \frac{v^j v^k}{2!} + \\ & + \left. \frac{\partial^3 \mathfrak{L}_{KL}}{\partial v^j \partial v^k \partial v^l} \right|_{\mathbf{v}=0} \frac{v^j v^k v^l}{3!} + \mathcal{O}(\mathbf{v}^4). \end{aligned}$$

Let us now examine the terms of the expansion up to the third order.

Concerning the first order term, S_{KL} must have a minimum on the diagonal $\mathbf{q}_{\text{in}} = \mathbf{q}_{\text{fin}}$ of $\Xi \times \Xi$. Therefore, recalling equations (3.18) and (3.10), and expressing the derivatives with respect to v^j by means of the derivatives with respect to q_{fin}^j , one has:

$$\left. \frac{\partial \mathfrak{L}_{KL}}{\partial v^j} \right|_{\mathbf{v}=0} = - \left. \frac{\partial S_{KL}}{\partial q_{\text{in}}^j} \right|_{\mathbf{q}_{\text{in}}=\mathbf{q}_{\text{fin}}} = 0. \quad (3.66)$$

This equation implies that \mathfrak{L}_{KL} is at least of second order in \mathbf{v} . Consequently, the analysis of the previous section for the functional dependence between \mathbf{v} and \mathbf{q}_{fin} stemming from the Euler-Lagrange equations can be analogously repeated in order to give the first order relation:

$$\left. \frac{\partial q_{\text{fin}}^j}{\partial v^j} \right|_{\mathbf{v}=0} = \delta_k^j. \quad (3.67)$$

This result, together with equations (3.10), (3.11) and (3.66), allows to see that the second order term of \mathfrak{L}_{KL} becomes:

$$\left. \frac{\partial^2 \mathfrak{L}_{KL}}{\partial v^j \partial v^k} \right|_{\mathbf{v}=0} = - \left. \frac{\partial^2 S_{KL}}{\partial q_{\text{fin}}^r \partial q_{\text{fin}}^j} \right|_{\mathbf{q}_{\text{in}}=\mathbf{q}_{\text{fin}}} \left. \frac{\partial q_{\text{fin}}^r}{\partial v^k} \right|_{\mathbf{v}=0} = g_{jk} \quad (3.68)$$

Once obtained the second-order term of the Lagrangian, one can proceed in the analysis of the functional dependence between \mathbf{v} and \mathbf{q}_{fin} and find that:

$$\left. \frac{\partial^2 q_{\text{fin}}^l}{\partial v^k \partial v^j} \right|_{\mathbf{v}=0} = -{}_g \Gamma_{jk}^l. \quad (3.69)$$

Consequently, the third order term of the Lagrangian is:

$$\begin{aligned} \left. \frac{\partial^3 \mathfrak{L}_{KL}}{\partial v^j \partial v^k \partial v^l} \right|_{\mathbf{v}=0} &= - \left. \frac{\partial^3 S_{KL}}{\partial q_{\text{fin}}^r \partial q_{\text{fin}}^n \partial q_{\text{fin}}^j} \right|_{\mathbf{q}_{\text{in}}=\mathbf{q}_{\text{fin}}} \left(\left. \frac{\partial q_{\text{fin}}^r}{\partial v^k} \frac{\partial q_{\text{fin}}^n}{\partial v^l} \right) \right|_{\mathbf{v}=0} + \\ &- \left. \frac{\partial^2 S_{KL}}{\partial q_{\text{fin}}^r \partial q_{\text{fin}}^j} \right|_{\mathbf{q}_{\text{in}}=\mathbf{q}_{\text{fin}}} \left. \frac{\partial^2 q_{\text{fin}}^r}{\partial v^l \partial v^k} \right|_{\mathbf{v}=0} = - \left. \frac{\partial^3 S_{KL}}{\partial q_{\text{fin}}^j \partial q_{\text{fin}}^k \partial q_{\text{fin}}^l} \right|_{\mathbf{q}_{\text{in}}=\mathbf{q}_{\text{fin}}} - {}_g \Gamma_{jkl} = -\frac{T_{jkl}}{2}, \end{aligned} \quad (3.70)$$

where, in the last equality, the following fact has been used:

$$\left. \frac{\partial^3 S_{KL}}{\partial q_{\text{fin}}^j \partial q_{\text{fin}}^k \partial q_{\text{fin}}^l} \right|_{\mathbf{q}_{\text{in}}=\mathbf{q}_{\text{fin}}} = {}_g \Gamma_{jkl} + \frac{T_{jkl}}{2}, \quad (3.71)$$

which is formula 4 of Lemma 2.1 in [56].

Collecting the results, one can write:

$$\mathfrak{L}_{KL} = \mathfrak{L}_{KL}|_{\mathbf{v}=0} + g_{jk} \frac{v^j v^k}{2!} - \frac{T_{jkl}}{2} \frac{v^j v^k v^l}{3!} + \mathcal{O}(\mathbf{v}^4), \quad (3.72)$$

from which it follows that, choosing $\alpha = -\frac{1}{2}$, the Lagrangian \mathfrak{L}_α differs from the third order approximation of \mathfrak{L}_{KL} only by the constant factor $\mathfrak{L}_{KL}|_{\mathbf{v}=0}$ as claimed. It would be very interesting to understand the conditions under which the Kullback-Leibler divergence of a given statistical model is the Hamilton principal function of some suitably-defined Lagrangian.

This appears to be relevant in the context of quantum information geometry of mixed states ([24] Chapter 7). Here, the quantum counterpart of

the Fisher-Rao metric has been studied extensively by Petz and coworkers ([58], [59] and references therein), who found that there is an infinite-number of metrics providing a meaningful generalization of the classical Fisher-Rao metric. Furthermore, unlike the classical case, there is no preferred definition for a skewness tensor T . This means that there is a good amount of freedom in the choice of a statistical structure on the space of quantum states. The usual way in which a statistical structure is defined is to start considering a generalization of some classical divergence function, and then derive a metric g and a tensor T on the space of quantum states. Interestingly, it is possible to use well known examples of quantum relative entropies as quantum divergence functions ([63]). As it is clear, in this quantum setting the statistical structure of the space of quantum states depends on the explicit form of the quantum divergence one starts with. Now, it has been shown above that the tensors g and T of a statistical manifold, being it classical or quantum, are completely encoded in the first four terms of the expansion of the Lagrangian associated with a divergence function, therefore, it is reasonable to argue that there must be some other geometrical informations hidden in the divergence function that are not fully captured by g and T alone. However the dynamical characterization of the quantum divergences stemming from the Hamilton-Jacobi approach outlined here can be fruitfully exploited to better understand the relations between the quantum divergences, the statistical structure they induce, and the geometrical structure of the space of quantum states.

Lastly this dynamical perspective naturally paves the way to an interesting interchange of tools and methods between information geometry and the theory of dynamical systems. For instance, the “unfolding-reduction” attitude towards dynamical systems clearly illustrated in [17] could be a powerful technique in the search of potential functions. Let us briefly comment on this point.

Let us consider a two dimensional sphere embedded into \mathbb{R}^3 through the map $i_{S^2} : \mathbb{S}^2 \rightarrow \mathbb{R}^3$. A local expression of this map is given by

$$\begin{cases} x^1 &= \sin \theta \cos \phi \\ x^2 &= \sin \theta \sin \phi \\ x^3 &= \cos \theta \end{cases}, \quad (3.73)$$

where $\theta \in]0, \pi[$ and $\phi \in]0, 2\pi[$. By means of this immersion it is possible to pull-back covariant tensors on \mathbb{R}^3 to \mathbb{S}^2 .

Let us consider the following statistical model: \mathbb{R}^3 equipped with the Euclidean metric $g = \delta_{jk} dx^j \otimes dx^k$ and the skewness tensor $T = dx^1 \otimes dx^1 \otimes dx^1 + dx^2 \otimes dx^2 \otimes dx^2 + dx^3 \otimes dx^3 \otimes dx^3$. According to the prescription outlined in previous section a canonical potential function is

$$S(x_{\text{in}}, x_{\text{fin}}) = \delta_{jk}(x_{\text{fin}}^j - x_{\text{in}}^j)(x_{\text{fin}}^k - x_{\text{in}}^k) + \frac{\alpha}{6} \left((x_{\text{fin}}^1 - x_{\text{in}}^1)^3 + (x_{\text{fin}}^2 - x_{\text{in}}^2)^3 + (x_{\text{fin}}^3 - x_{\text{in}}^3)^3 \right).$$

By means of the previous immersion one can pull back this potential to \mathbb{S}^2 obtaining the following function

$$S_{\mathbb{S}^2}((\theta_0, \phi_0), (\theta_1, \phi_1)) = \frac{1}{2} (\sin \theta_0 \sin \theta_1 \cos(\phi_1 - \phi_0) + \cos \theta_0 \cos \theta_1) + \frac{\alpha}{6} \left((\sin \theta_0 \cos \phi_0 - \sin \theta_1 \cos \phi_1)^3 + (\sin \theta_0 \sin \phi_0 - \sin \theta_1 \sin \phi_1)^3 + (\cos \theta_0 - \cos \theta_1)^3 \right).$$

A direct computation shows that this is a potential function on the submanifold \mathbb{S}^2 and it generates a metric tensor $g_{\mathbb{S}^2}$ and a skewness tensor $T_{\mathbb{S}^2}$ which coincide with the pull-back to \mathbb{S}^2 of the metric and skewness tensors on \mathbb{R}^3 . Indeed

$$g_{\mathbb{S}^2} = d\theta \otimes d\theta + (\sin \theta)^2 d\phi \otimes d\phi, \quad (3.74)$$

$$\begin{aligned} T_{\mathbb{S}^2} = & - (\cos^3 \phi \cos^3 \theta + \sin^3 \phi \cos^3 \theta - \sin^3 \theta) d\theta \otimes d\theta \otimes d\theta - \\ & - \cos^2 \theta \sin \theta \sin \phi \cos \phi (\cos \phi - \sin \phi) d\theta \otimes d\theta \otimes d\phi + \\ & + \sin^2 \theta \cos \theta \sin \phi \cos \phi (\cos \phi + \sin \phi) d\theta \otimes d\phi \otimes d\phi + \\ & + \sin^3 \theta (\sin^3 \phi - \cos^3 \phi) d\phi \otimes d\phi \otimes d\phi. \end{aligned} \quad (3.75)$$

This simple example shows that in some cases it is possible to obtain a tensor which is no more constant, the metric tensor on the sphere, starting from an Euclidean space, and the potential on the Euclidean space induces a potential on the submanifold. However one could also invert this procedure. If one starts from a manifold with a non constant tensor it is possible to enlarge this manifold to a larger space equipped with a constant metric tensor: this is the meaning of the word “unfolding” in such a context.

Conclusions and Outlooks

Hamilton-Jacobi theory and the theory of canonical transformations are the central themes of this thesis which allow to put in contact all the topics which have been discussed in the previous pages. First chapter has been devoted to Quantum Mechanics, the second has focused on covariant description of particles and fields mechanics whereas the subject of last chapter has been information theory. Different motivations have suggested to investigate the role of these geometrical methods in all these distinct situations, leading to the results presented in the previous chapters.

The connection between Hamilton-Jacobi theory and Quantum Mechanics roots back to the foundations: Bohr and Sommerfeld, for instance, introduced the first quantization rules by looking at action-angle variables of completely integrable systems. Furthermore WKB method has shown the connection between phases of wave functions and solutions of suitable Hamilton-Jacobi equations. However in this chapter two different aspects have been accented. From one side it has been presented how to define classical-like completely integrable dynamics by reducing a quantum systems to a subset of states which has a manifold structure. We could summarize as follows: “dequantization” as a reduction procedure from linear to nonlinear evolution, along with a “quantization” considered as an unfolding procedure to associate a linear system out of a nonlinear one. On the other hand various attempts of defining variational formulation of a Quantum dynamics have been illustrated, both in particle and fields dynamics. Here a “Langrangian-like” formulation allows for a covariant description which avoids the splitting into time and space.

As far as covariant description of fields dynamics is concerned we limited our analysis to a more geometrical interpretation of Peierls bracket. Since this bracket involves fields evaluated at different space-time points, it has been reasonable to investigate the relationship between this formulation and the one obtained through a canonical transformation from $T^*\mathcal{M}$ to $\mathcal{M} \times \mathcal{M}$, as the one generated by Hamilton principal function (7).

Similarly divergence functions in information theory share some of the

the properties characterizing Hamilton principal functions. Indeed in the last chapter we have shown that actually a potential function can be obtained as the Hamilton principal function associated with a given dynamical system built out of the geometrical ingredient contained in a statistical model.

Of course the results presented in this thesis are not the end of the story. Many questions can now be raised and further investigations related to the contents of the previous chapters would be interesting from many points of view.

For instance the relationship between divergence functions and Hamilton principal functions permits the introduction of techniques coming from Lagrangian mechanics in information theory. This might also lead to a new way of interpreting relative entropies according to a more dynamical perspective. Perhaps one could use relative entropies to formulate proper variational principle relevant for thermodynamics instead of thermostatic.

As far as Peierls bracket is concerned new developments are now allowed. From one side one should better understand what happens if the action functional may not be written in terms of a density. From another side it would be very interesting to have a deeper look at the relationship between contact structures and constrained dynamical systems, in particular gauge theories.

Finally, the idea of using systems of Hamilton-Jacobi equations seems to be interesting in order to preserve covariance. Further investigations are necessary in order to understand its applicability in the case of general relativity and a comparison with the approach by Bergmann and Komar, briefly outlined in the introduction, could be helpful to achieve this goal.

Appendix A: A Short Introduction to the Geometry of First Jet Bundles

In this appendix we will introduce some basic notions on the geometric structures which characterize the first jet bundle J^1E which we have employed throughout the second chapter of this thesis. The contents of this appendix are collected from the book [64].

Let us consider a fibre bundle $\pi : E \rightarrow \mathcal{M}$ and a point $p \in \mathcal{M}$. Let ψ, ϕ be two local sections of the bundle E . ψ and ϕ are said to be 1-equivalent at p iff

$$\phi(p) = \psi(p) \tag{3.76}$$

$$\left. \frac{\partial \phi^a}{\partial x^\mu} \right|_p = \left. \frac{\partial \psi^a}{\partial x^\mu} \right|_p, \tag{3.77}$$

for some adapted coordinate system (u^a, x^μ) . The equivalence class containing ϕ is called the 1-jet of ϕ at p and it is denoted by $j_p^1\phi$.

Even if this definition is based on the use of local section, the equivalence relation is not influenced by the given choice of coordinate system. Indeed the following lemma is valid:

Lemma 1 *Lemma Let (E, π, \mathcal{M}) be a bundle and $p \in \mathcal{M}$. Suppose that the two sections ϕ, ψ satisfy $\phi(p) = \psi(p)$. Let (x^μ, u^a) and (y^ν, v^b) two coordinate system around $\phi(p)$. If*

$$\left. \frac{\partial u^a \circ \phi}{\partial x^\mu} \right|_p = \left. \frac{\partial u^a \circ \psi}{\partial x^\mu} \right|_p,$$

$\forall 1 \leq \mu \leq m$ and $\forall 1 \leq a \leq n$, then

$$\left. \frac{\partial v^b \circ \phi}{\partial y^\nu} \right|_p = \left. \frac{\partial v^b \circ \psi}{\partial y^\nu} \right|_p.$$

Proof 1 *From the chain rule and the hypotheses it follows that:*

$$\begin{aligned} \left. \frac{\partial v^b \circ \phi}{\partial y^\nu} \right|_p &= \left. \frac{\partial v^b \circ \phi}{\partial x^\mu} \right|_p \left. \frac{\partial x^\mu}{\partial y^\nu} \right|_p = \left(\left. \frac{\partial v^b}{\partial x^\mu} \right|_{\phi(p)} + \left. \frac{\partial v^b}{\partial u^a} \right|_{\phi(p)} \left. \frac{\partial u^a \circ \phi}{\partial x^\mu} \right|_p \right) \left. \frac{\partial x^\mu}{\partial y^\nu} \right|_p = \\ &= \left(\left. \frac{\partial v^b}{\partial x^\mu} \right|_{\psi(p)} + \left. \frac{\partial v^b}{\partial u^a} \right|_{\psi(p)} \left. \frac{\partial u^a \circ \psi}{\partial x^\mu} \right|_p \right) \left. \frac{\partial x^\mu}{\partial y^\nu} \right|_p = \left. \frac{\partial v^b \circ \psi}{\partial y^\nu} \right|_p. \end{aligned} \quad (3.78)$$

In reference [64] it is proven that the set J^1E of all 1-jets of sections of E form a finite-dimensional smooth manifold and an atlas on J^1E can be constructed in terms of an atlas on the bundle E .

Definition 1 *Let (E, π, \mathcal{M}) be a bundle and let (U, u) be an adapted coordinate system on E where $u = (x^\mu, u^a)$. The induced coordinate system (U^1, u^1) on J^1E is defined as*

$$\begin{aligned} U^1 &= \{j_p^1\phi : \phi(p) \in U\} \\ u^1 &= (x^\mu, u^a, u_\mu^a) \end{aligned}$$

where $x^\mu(j_p^1\phi) = x^\mu(p)$, $u^a(j_p^1\phi) = u^a(\phi(p))$ and $u_\mu^a(j_p^1\phi) = \left. \frac{\partial \phi^a}{\partial x^\mu} \right|_p$.

Furthermore it is possible to equip this manifold with two structures of fibre bundles, one with base manifold E , the other with base manifold \mathcal{M} . These two bundle structures are given in terms of the following surjective projections:

$$\begin{aligned} \pi_{1,0} : J^1E &\rightarrow E \\ j_p^1\phi &\rightarrow \phi(p) \end{aligned}$$

and

$$\begin{aligned} \pi_1 : J^1E &\rightarrow \mathcal{M} \\ j_p^1\phi &\rightarrow p \end{aligned}$$

In particular it is possible to prove the following theorems (a proof is contained in [64]):

Theorem 1 *The triple $(J^1E, \pi_{1,0}, E)$ can be given the structure of an affine bundle modelled on the vector bundle $\pi^*(T^*\mathcal{M}) \otimes VE^5$ over the base manifold E , in such a way that for each adapted chart (U, u) on E the map*

$$\begin{aligned} t_u : \pi_{1,0}^{-1}(U) &\rightarrow U \times \mathbb{R}^{nm} \\ j_p^1\phi &\rightarrow (\phi(p), u_\mu^a(j_p^1\phi)) \end{aligned}$$

is an affine local trivialisation.

⁵The space VE is the space of vertical tangent vectors to the bundle E .

Theorem 2 *If (E, π, \mathcal{M}) is a bundle, then $(J^1E, \pi_1, \mathcal{M})$ is a bundle.*

Example 1 *Let us consider the trivial bundle $E = \mathbb{R}^2 \times \mathbb{R}$, with global coordinates $(x^1, x^2; u)$. The corresponding global coordinates on J^1E are $(x^1, x^2; u; u_1, u_2)$. To each 1-jet $j_p^1\phi$ where $p = (p^1, p^2) \in \mathbb{R}^2$ there corresponds an inhomogeneous linear map $\bar{\psi} : \mathbb{R}^2 \rightarrow \mathbb{R}$ defined as follows:*

$$\bar{\psi}(q) = \phi(p) + u_1(j_p^1\phi)(q^1 - p^1) + u_2(j_p^1\phi)(q^2 - p^2). \quad (3.79)$$

It is possible to associate to the map $\bar{\psi}$ a section $\psi = (id_{\mathbb{R}^2}, \bar{\psi})$ of the bundle E and from the definition it is easy to verify that $j_p^1\phi = j_p^1\psi$. Therefore the jet $j_p^1\phi$ is a coordinate-free construction which contains the same information on the derivatives of a section ϕ as its first order Taylor polynomial $\bar{\psi}$.

Example 2 *Let E be the trivial bundle $\mathbb{R} \times \mathcal{M}$ with local coordinate functions given by $(t; q^a)$. Sections of this bundle are curves of \mathcal{M} and consequently the first jet $j_{t_0}^1\gamma$ of a curve γ is a tangent vector of the point $\gamma(t_0)$. Therefore the manifold $J^1E \simeq \mathbb{R} \times T\mathcal{M}$, where $T\mathcal{M}$ is the tangent bundle to the manifold \mathcal{M} . A set of coordinate functions of J^1E are written as $(t; q^a; \dot{q}^a)$.*

With this interpretation a section Φ of the bundle $(J^1E, \pi_{1,0}, E)$ can be interpreted as a vector field on E and has coordinate representation

$$\Phi = X^a(t, q^a) \frac{\partial}{\partial q^a}.$$

Corresponding to each local section ϕ of the bundle (E, π, \mathcal{M}) there is a uniquely determined local section of the bundle $(J^1E, \pi_1, \mathcal{M})$ which is called the first prolongation $j^1\phi$ of the field ϕ .

Definition 2 *Given the bundle (E, π, \mathcal{M}) and a local section ϕ of E , the first prolongation $j^1\phi$ of ϕ is the local section of the bundle $(J^1E, \pi_1, \mathcal{M})$ defined by*

$$j^1\phi(p) = j_p^1\phi.$$

It is possible to define the first prolongation of bundle morphisms of first jet bundles over diffeomorphic manifolds: this is related to the description of point symmetries in Lagrangian mechanics. However we will not enter into these details because we have not used these concepts in chapter 2.

Example 3 *Let E be the trivial bundle $(E = \mathbb{R}^2 \times \mathbb{R}, pr_1, \mathbb{R}^2)$ with coordinates $(x^1, x^2; u)$. If a section ϕ is defined as*

$$\phi(x^1, x^2) = (x^1, x^2; x^1 \sin x^2)$$

then the first prolongation $j^1\phi$ is written as

$$j^1\phi(x^1, x^2; x^1 \sin x^2, \sin x^2, x^1 \cos x^2).$$

Analogously it is possible to associate to a vector field X on E the first prolongation X^1 of X which is a vector field on the first jet bundle J^1E . It is possible to interpret this construction as the infinitesimal version of the first prolongation of a section and more generally of a suitable bundle morphism. However in this appendix we will consider only the first prolongation of vertical vector fields. For more details see [64].

Let us start from the two bundles $(J^1E, \pi_1, \mathcal{M})$ and $(VE, \nu_\pi, \mathcal{M})$. The vertical bundle $(VJ^1E, \nu_{\pi_1}, \mathcal{M})$ of the former and the first jet bundle $(J^1VE, (\nu_\pi)_1, \mathcal{M})$ of the latter are canonically diffeomorphic.

Theorem 3 *There is a canonical diffeomorphism $i_1 : J^1VE \rightarrow VJ^1E$ which projects to the identity on \mathcal{M} .*

The coordinate correspondence between J^1VE and VJ^1E can be given as follows. An element ξ in VJ^1E can be written as

$$\xi = \xi^a \frac{\partial}{\partial u^a} \Big|_{j_p^1 \phi} + \xi_\mu^a \frac{\partial}{\partial u_\mu^a} \Big|_{j_p^1 \phi} .$$

The corresponding element in J^1VE is written in terms of a section ϕ of E and a vertical vector field over E satisfying $i_1(j_p^1(X \circ \phi)) = \xi$. in coordinate

$$j_p^1(X \circ \phi) = \left(p; X^a(\phi(p)), \frac{d}{dx^\mu} X^a(\phi(p)) \Big|_{j_p^1 \phi} \right)$$

where $\frac{dX^a}{dx^\mu} \Big|_{j_p^1 \phi} = \frac{\partial X^a}{\partial x^\mu} \Big|_{\phi(p)} + u_\mu^b(j^1 \phi) \frac{\partial X^a}{\partial u^b} \Big|_{\phi(p)}$ is called the total derivative of X^a . Therefore the coordinate representation of the diffeomorphism i_1 is $\xi^a = X^a(\phi(p))$ and $\xi_\mu^a = \frac{dX^a}{dx^\mu} \Big|_{j_p^1 \phi}$.

The diffeomorphism i_1 can be used to prolong vertical vector field on E to give vertical vector field on J^1E . So suppose that X is a vertical vector field on E ; the pair $(X, id_{\mathcal{M}})$, where $id_{\mathcal{M}}$ is the identity map on \mathcal{M} , can be seen as a bundle morphism between (E, π, \mathcal{M}) and $(VE, \nu_\pi, \mathcal{M})$. Therefore the first prolongation of this bundle morphism is the map $j^1X : J^1E \rightarrow J^1VE$ and the map $i_1 \circ j^1X$ is a map from J^1E to VJ^1E . Therefore $i_1 \circ j^1X$ defines a vertical vector field X^1 on J^1E .

If $X = X^a \frac{\partial}{\partial u^a}$ then

$$X^1 = X^a \frac{\partial}{\partial u^a} + \frac{dX^a}{dx^\mu} \frac{\partial}{\partial u_\mu^a}$$

and if γ is the flow of X , $j^1\gamma$ (defined as $j^1\gamma(p, t) = j_p^1\gamma_t$) is the flow of X^1 .

A final operation on the jet bundle J^1E that we will introduce in this appendix is the notion of vertical lift. Starting from a covector $\eta \in T^*\mathcal{M}$ and a vertical tangent vector ζ on E it is possible to define a vertical vector tangent to the bundle $(J^1E, \pi_{1,0}, \mathcal{E})$. This is the content of the following theorem:

Theorem 4 *Let us consider a point $j_p^1\phi \in J^1E$, a covector $\eta \in T_p^*\mathcal{M}$ and a vertical tangent vector $\zeta \in V_{\phi(p)}E$. Let W be a neighbourhood of $p \in \mathcal{M}$ and let $\gamma : W \times \mathbb{R} \rightarrow E$ satisfy $[t \rightarrow \gamma(p, t)] = \zeta^6$ and $j_p^1(q \rightarrow \gamma(q, 0)) = j_p^1\phi$. Let $f \in C^\infty(\mathcal{M})$ satisfy $f(p) = 0$ and $df_p = \eta$. Then the new tangent vector*

$$[t \rightarrow j_p^1(q \rightarrow \gamma(q, tf(q)))]$$

denoted by $\eta \bullet_{j_p^1\phi} \zeta$ is a vertical tangent vector on J^1E which does not depend on the choice of f and γ .

If $\eta = \eta_\mu dx^\mu$ and $\zeta = \zeta^a \frac{\partial}{\partial u^a}$ the vertical tangent vector $\eta \bullet_{j_p^1\phi} \zeta$ can be written as

$$\eta \bullet_{j_p^1\phi} \zeta = \eta_\mu \zeta^a \frac{\partial}{\partial u_\mu^a}. \quad (3.80)$$

From this vertical lift operation it is possible to define a vector-valued one-form S_ω which associates with a tangent vector $\xi \in T_{j_p^1\phi}J^1E$ a canonical vertical tangent vector $S_\omega(\xi)$. The definition of this canonical vertical tangent vector requires the introduction of other elements which are not necessary for the following discussion and consequently we will give directly the expression of S_ω in a coordinate system; for more details see [64]. The vector-valued one form S_ω can be written as follows:

$$S_\omega = \omega_\nu (u^\nu - u_\mu^\nu dx^\mu) \otimes \frac{\partial}{\partial u_\nu^a}, \quad (3.81)$$

where $\omega = \omega_\mu dx^\mu$ is a one-form on \mathcal{M} . In order to avoid the explicit dependence on the one-form ω one can introduce a new tensor field S of type $(2, 1)$ such that

$$C(S \otimes \omega) = S_\omega$$

where $C(S \otimes \omega)$ denotes the contraction of the the tensor $S \otimes \omega$. However, when \mathcal{M} is orientable with a given volume form Ω it is possible to replace the tensor S with a vector-valued m-form

$$S_\Omega = C(S \otimes \Omega), \quad (3.82)$$

⁶The symbol $[\gamma(t)]$ denotes the equivalence class of curves which γ belongs to and consequently defines a tangent vector.

which in coordinates can be written as

$$S_\Omega = (u^a - u_\mu^a dx^\mu) \wedge i_{\partial_\nu} \Omega \otimes \frac{\partial}{\partial u_\nu^a}.$$

This vector-valued m-form allows to recover the vector-valued one-form S_ω and therefore the definition of vertical lift.

Appendix B: Basic Definitions on Contact Manifolds

Contact manifolds are usually presented as the odd-dimensional counterpart of symplectic manifolds. If one looks from the dual point of view of functions [65], the space of functions on a symplectic manifold can be equipped with a canonical Poisson bracket whereas the space of functions on a contact manifold can be endowed with a “natural” Jacobi bracket. The unique role of the Jacobi bracket originates from a theorem by Kirillov which examines the most general Lie bracket one may define on the algebra of functions when an additional locality requirement is assumed, locality meaning that $\text{supp}([f, g]) \subseteq \text{supp}(f) \cap \text{supp}(g)$. Let us begin with some definitions.

On some $(2n + 1)$ -dimensional manifold \mathcal{M} , a differential form θ defines a contact structure if $\theta \wedge (d\theta)^n \neq 0$, i.e., it is a volume element. However if one multiplies such a form by a never vanishing function the result is another one form satisfying the same condition. Therefore a contact structure is actually defined as an equivalence class of one forms related by multiplication by a never vanishing function. By means of this contact one form hyperplanes of the tangent space to the manifold which are called contact elements are selected (for more details see Ref. [32]).

This arbitrariness may be reduced by imposing invariance requirements, for instance invariance with respect to the Poincaré group.

A manifold \mathcal{M} endowed with a contact structure, is called a contact manifold. Given a contact manifold it is possible to define a Lie algebra structure on the space of functions by means of the following formula

$$[f, g] \theta \wedge (d\theta)^n = (n - 1)df \wedge dg \wedge \theta \wedge (d\theta)^{n-1} + (fdg - gdf) \wedge (d\theta)^n. \quad (3.83)$$

This bracket is clearly local by construction, and satisfies the Jacobi identity

$$[f, [g, h]] = [[f, g], h] + [g, [f, h]]$$

which expresses the property of defining a derivation of the Lie product. It should be stressed that the bracket only depends on the one form. Therefore it will possess all the invariance properties enjoyed by θ .

To make contact with the usual definition of Jacobi bracket one defines a vector field Γ (also called Reeb vector field) and a bivector field Λ with the help of θ and $d\theta$, satisfying the following properties

$$i_{\Gamma}\theta \wedge (d\theta)^n = (d\theta)^n \quad (3.84)$$

$$i_{\Lambda}\theta \wedge (d\theta)^n = n\theta \wedge (d\theta)^{n-1}. \quad (3.85)$$

Previous bracket may be given now in the more conventional form by setting

$$[f, g] = \Lambda(df, dg) + fL_{\Gamma}g - gL_{\Gamma}f, \quad (3.86)$$

where L_{Γ} stays for the Lie derivative along Γ . Jacobi identity in this case corresponds to the following requirements on the pair (Λ, Γ) :

$$[\Lambda, \Lambda]_S = 2\Gamma \wedge \Lambda \quad (3.87)$$

$$L_{\Gamma}\Lambda = 0 \quad (3.88)$$

where the bracket $[\cdot, \cdot]_S$ is the Schouten brackets on the algebra of multivectors on a manifold (see Ref. [66]).

Any function is associated with a first-order differential operator

$$\tilde{X}_f = \Lambda(df, \cdot) + f\Gamma - L_{\Gamma}f,$$

and it is worth pointing out that the identity function is not mapped onto 0 but gives the vector field Γ .

Notice that Leibniz rule is replaced by

$$[f, gh] = [f, g]h + g[f, h] - [f, 1]gh$$

which explains the difference between Jacobi brackets and Poisson brackets. This generalized Leibniz rule says that the bracket is actually associated with a bidifferential operator instead of a bivector field like in the case of the Poisson brackets.

In general one defines the Hamiltonian vector field, X_f , associated with the function f , to be the vector field

$$X_f = \Lambda(df, \cdot) + f\Gamma, \quad (3.89)$$

and this association is a homomorphism of Lie algebra, i.e.

$$[X_f, X_g] = X_{[f, g]}.$$

On the subalgebra of functions f such that $L_{\Gamma}f = 0$, the Jacobi bracket becomes a Poisson Bracket.

Eventually let us notice that the definition (3.86) of a Jacobi structure by means of a bivector field Λ and a vector field Γ satisfying properties (3.87) and (3.88) is independent from the existence of a underlying contact manifold. It is worth noticing that this definition also shows that a Jacobi bracket is unrelated to the dimensions of the manifold.

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