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From Tools in Symplectic and Poisson Geometry to Souriau's theories of Statistical Mechanics and Thermodynamics

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Abstract

I present in this paper some tools in Symplectic and Poisson Geometry in view of their applications in Geometric Mechanics and Mathematical Physics. After a short discussion of the Lagrangian and Hamiltonian formalisms, including the use of symmetry groups, and a presentation of the Tulczyjew's isomorphisms (which explain some aspects of the relations between these formalisms), I explain the concept of manifold of motions of a mechanical system and its use, due to J.-M. Souriau, in Statistical Mechanics and Thermodynamics. The generalization of the notion of thermodynamic equilibrium in which the one-dimensional group of time translations is replaced by a multi-dimensional, maybe non-commutative Lie group, is discussed and examples of applications in Physics are given.

1 Introduction

1.1 Contents of the paper, sources and further reading

This paper presents tools in Symplectic and Poisson Geometry in view of their application in Geometric Mechanics and Mathematical Physics. The Lagrangian formalism and symmetries of Lagrangian systems are discussed in Sections 2 and 3, the Hamiltonian formalism and symmetries of Hamiltonian systems in Sections 4 and 5. Section 6 introduces the concepts of Gibbs state and of thermodynamic equilibrium of a mechanical system, and presents several examples. For a monoatomic classical ideal gas, eventually in a gravity field, or a monoatomic relativistic gas the Maxwell-Boltzmann and Maxwell-Jüttner probability distributions are derived. The Dulong and Petit law which governs the specific heat of solids is obtained. Finally Section 7 presents the generalization of the concept of Gibbs state, due to Jean-Marie Souriau, in which the group of time translations is replaced by a (multi-dimensional and eventually non-Abelian) Lie group.

Several books [1, 2, 12, 15, 18, 19, 30, 31, 45, 63] discuss, much more fully than in the present paper, the contents of Sections 2 to 5. The interested reader is referred to these books for detailed proofs of results whose proofs are only briefly sketched here. The recent paper [38] contains detailed proofs of most results presented here in Sections 4 and 5.

The main sources used for Sections 6 and 7 are the book and papers by Jean-Marie Souriau [55, 54, 56, 57, 58] and the beautiful small book by G. W. Mackey [34].

The Euler-Poincaré equation, which is presented with Lagrangian symmetries at the end of Section 3, is not really related to symmetries of a Lagrangian system, since the Lie algebra which acts on the configuration space of the system is not a Lie algebra of symmetries of the Lagrangian. Moreover in its intrinsic form that equation uses the concept of Hamiltonian momentum map presented later, in Section 5. Since the Euler-Poincaré equation is not used in the following sections, the reader can skip the corresponding subsection at his or her first reading.

1.2 Notations

The notations used are more or less those generally used now in Differential Geometry. The tangent and cotangent bundles to a smooth manifold M are denoted by TM and T^*M , respectively, and their canonical projections by $\tau_M : TM \rightarrow M$ and $\pi_M : T^*M \rightarrow M$. The vector spaces of k -multivectors and k -forms on M are denoted by $A^k(M)$ and $\Omega^k(M)$, respectively, with $k \in \mathbb{Z}$ and, of course, $A^k(M) = \{0\}$ and $\Omega^k(M) = \{0\}$ if $k < 0$ and if $k > \dim M$, k -multivectors and k -forms being skew-symmetric. The exterior algebras of multivectors and forms of all degrees are denoted by $A(M) = \bigoplus_k A^k(M)$ and $\Omega(M) = \bigoplus_k \Omega^k(M)$, respectively. The exterior differentiation operator of differential forms on a smooth manifold M is denoted by $d : \Omega(M) \rightarrow \Omega(M)$. The interior product of a differential form $\eta \in \Omega(M)$ by a vector field $X \in A^1(M)$ is denoted by $i(X)\eta$.

Let $f : M \rightarrow N$ be a smooth map defined on a smooth manifold M , with values in another smooth manifold N . The pull-back of a form $\eta \in \Omega(N)$ by a smooth map $f : M \rightarrow N$ is denoted by $f^*\eta \in \Omega(M)$.

A smooth, time-dependent vector field on the smooth manifold M is a smooth map $X : \mathbb{R} \times M \rightarrow TM$ such that, for each $t \in \mathbb{R}$ and $x \in M$, $X(t, x) \in T_x M$, the vector space tangent to M at x . When, for any $x \in M$, $X(t, x)$ does not depend on $t \in \mathbb{R}$, X is a smooth vector field in the usual sense, *i.e.*, an element in $A^1(M)$. Of course a time-dependent vector field can be defined on an open subset of $\mathbb{R} \times M$ instead than on the whole $\mathbb{R} \times M$. It defines a differential equation

$$\frac{d\varphi(t)}{dt} = X(t, \varphi(t)), \quad (*)$$

said to be *associated* to X . The (full) *flow* of X is the map Ψ^X , defined on an open subset of $\mathbb{R} \times \mathbb{R} \times M$, taking its values in M , such that for each $t_0 \in \mathbb{R}$ and $x_0 \in M$ the parametrized curve $t \mapsto \Psi^X(t, t_0, x_0)$ is the maximal integral curve of $(*)$ satisfying $\Psi(t_0, t_0, x_0) = x_0$. When t_0 and $t \in \mathbb{R}$ are fixed, the map $x_0 \mapsto \Psi^X(t, t_0, x_0)$ is a diffeomorphism, defined on an open subset of M (which may be empty) and taking its values in another open subset of M , denoted by $\Psi_{(t, t_0)}^X$. When X is in fact a vector field in the usual sense (not dependent on time), $\Psi_{(t, t_0)}^X$ only depends on $t - t_0$. Instead of the full flow of X we can use its *reduced flow* Φ^X , defined on an open subset of $\mathbb{R} \times M$ and taking its values in M , related to the full flow Ψ^X by

$$\Phi^X(t, x_0) = \Psi^X(t, 0, x_0), \quad \Psi^X(t, t_0, x_0) = \Phi^X(t - t_0, x_0).$$

For each $t \in \mathbb{R}$, the map $x_0 \mapsto \Phi^X(t, x_0) = \Psi^X(t, 0, x_0)$ is a diffeomorphism, denoted by Φ_t^X , defined on an open subset of M (which may be empty) onto another open subset of M .

When $f : M \rightarrow N$ is a smooth map defined on a smooth manifold M , with values in another smooth manifold N , there exists a smooth map $Tf : TM \rightarrow TN$ called the *prolongation of f to vectors*, which for each fixed $x \in M$ linearly maps $T_x M$ into $T_{f(x)} N$. When f is a diffeomorphism of M onto N , Tf is an isomorphism of TM onto TN . That property allows us to define the *canonical lifts* of a vector field X in $A^1(M)$ to the tangent bundle TM and to the cotangent bundle T^*M . Indeed, for each $t \in \mathbb{R}$, Φ_t^X is a diffeomorphism of an open subset of M onto another open subset of M . Therefore $T\Phi_t^X$ is a diffeomorphism of an open subset of TM onto another open subset of TM . It turns out that when t takes all possible values in \mathbb{R} the set of all diffeomorphisms $T\Phi_t^X$ is the reduced flow of a vector field \bar{X} on TM , which is the *canonical lift* of X to the tangent bundle TM .

Similarly, the transpose $(T\Phi_{-t}^X)^T$ of $T\Phi_{-t}^X$ is a diffeomorphism of an open subset of the cotangent bundle T^*M onto another open subset of T^*M , and when t takes all possible values in \mathbb{R} the set of all diffeomorphisms $(T\Phi_{-t}^X)^T$ is the reduced flow of a vector field \hat{X} on T^*M , which is the *canonical lift* of X to the cotangent bundle T^*M .

The canonical lifts of a vector field to the tangent and cotangent bundles are used in Sections 3 and 5. They can be defined too for time-dependent vector fields.

2 The Lagrangian formalism

2.1 The configuration space and the space of kinematic states

The principles of Mechanics were stated by the great English mathematician *Isaac Newton* (1642–1727) in his book *Philosophia Naturalis Principia Mathematica* published in 1687 [44]. On this basis, a little more than a century later, *Joseph Louis Lagrange* (1736–1813)

in his book *Mécanique analytique* [28] derived the equations (today known as the *Euler-Lagrange equations*) which govern the motion of a mechanical system made of any number of material points or rigid material bodies interacting between them by very general forces, and eventually submitted to external forces.

In modern mathematical language, these equations are written on the *configuration space* and on the *space of kinematic states* of the considered mechanical system. The *configuration space* is a smooth n -dimensional manifold N whose elements are all the possible configurations of the system (a configuration being the position in space of all parts of the system). The *space of kinematic states* is the tangent bundle TN to the configuration space, which is $2n$ -dimensional. Each element of the space of kinematic states is a vector tangent to the configuration space at one of its elements, *i.e.* at a configuration of the mechanical system, which describes the velocity at which this configuration changes with time. In local coordinates a configuration of the system is determined by the n coordinates x^1, \dots, x^n of a point in N , and a kinematic state by the $2n$ coordinates $x^1, \dots, x^n, v^1, \dots, v^n$ of a vector tangent to N at some element in N .

2.2 The Euler-Lagrange equations

When the mechanical system is *conservative*, the Euler-Lagrange equations involve a single real valued function L called the *Lagrangian* of the system, defined on the product of the real line \mathbb{R} (spanned by the variable t representing the time) with the manifold TN of *kinematic states* of the system. In local coordinates, the Lagrangian L is expressed as a function of the $2n + 1$ variables, $t, x^1, \dots, x^n, v^1, \dots, v^n$ and the Euler-Lagrange equations have the remarkably simple form

$$\frac{d}{dt} \left(\frac{\partial L}{\partial v^i}(t, x(t), v(t)) \right) - \frac{\partial L}{\partial x^i}(t, x(t), v(t)) = 0, \quad 1 \leq i \leq n,$$

where $x(t)$ stands for $x^1(t), \dots, x^n(t)$ and $v(t)$ for $v^1(t), \dots, v^n(t)$ with, of course,

$$v^i(t) = \frac{dx^i(t)}{dt}, \quad 1 \leq i \leq n.$$

2.3 Hamilton's principle of stationary action

The great Irish mathematician *William Rowan Hamilton* (1805–1865) observed [16, 17] that the Euler-Lagrange equations can be obtained by applying the standard techniques of *Calculus of Variations*, due to *Leonhard Euler* (1707–1783) and *Joseph Louis Lagrange*, to the *action integral*¹

$$I_L(\gamma) = \int_{t_0}^{t_1} L(t, x(t), v(t)) dt, \quad \text{with } v(t) = \frac{dx(t)}{dt},$$

where $\gamma: [t_0, t_1] \rightarrow N$ is a smooth curve in N parametrized by the time t . These equations express the fact that the action integral $I_L(\gamma)$ is *stationary* with respect to any smooth infinitesimal variation of γ with fixed end-points $(t_0, \gamma(t_0))$ and $(t_1, \gamma(t_1))$. This fact is today called *Hamilton's principle of stationary action*. The reader interested in *Calculus of Variations* and its applications in *Mechanics and Physics* is referred to the books [8, 10, 29].

¹Lagrange observed that fact before Hamilton, but in the last edition of his book he chose to derive the Euler-Lagrange equations by application of the *principle of virtual works*, using a very clever evaluation of the virtual work of inertial forces for a smooth infinitesimal variation of the motion.

2.4 The Euler-Cartan theorem

The *Lagrangian formalism* is the use of Hamilton's principle of stationary action for the derivation of the equations of motion of a system. It is widely used in Mathematical Physics, often with more general Lagrangians involving more than one independent variable and higher order partial derivatives of dependent variables. For simplicity I will consider here only the Lagrangians of (maybe time-dependent) conservative mechanical systems.

An intrinsic geometric expression of the Euler-Lagrange equations, which does not use local coordinates, was obtained by the great French mathematician *Élie Cartan* (1869–1951). Let us introduce the concepts used by the statement of this theorem.

2.4.1 Definitions. Let N be the configuration space of a mechanical system and let its tangent bundle TN be the space of kinematic states of that system. We assume that the evolution with time of the state of the system is governed by the Euler-Lagrange equations for a smooth, maybe time-dependent Lagrangian $L : \mathbb{R} \times TN \rightarrow \mathbb{R}$.

1. The cotangent bundle T^*N is called the *phase space* of the system.
2. The map $\mathcal{L}_L : \mathbb{R} \times TN \rightarrow T^*N$

$$\mathcal{L}_L(t, v) = d_{\text{vert}}L(t, v), \quad t \in \mathbb{R}, v \in TN,$$

where $d_{\text{vert}}L(t, v)$ is the *vertical differential* of L at (t, v) , i.e. the differential at v of the map $w \mapsto L(t, w)$, with $w \in \tau_N^{-1}(\tau_N(v))$, is called the *Legendre map* associated to L .

3. The map $E_L : \mathbb{R} \times TN \rightarrow \mathbb{R}$ given by

$$E_L(t, v) = \langle \mathcal{L}_L(t, v), v \rangle - L(t, v), \quad t \in \mathbb{R}, v \in TN,$$

is called the *energy function* associated to L .

4. The 1-form on $\mathbb{R} \times TN$

$$\widehat{\omega}_L = \mathcal{L}_L^* \theta_N - E_L(t, v) dt,$$

where θ_N is the Liouville 1-form on T^*N , is called the *Euler-Poincaré* 1-form.

2.4.2 Theorem (Euler-Cartan theorem). *A smooth curve $\gamma : [t_0, t_1] \rightarrow N$ parametrized by the time $t \in [t_0, t_1]$ is a solution of the Euler-Lagrange equations if and only if, for each $t \in [t_0, t_1]$ the derivative with respect to t of the map $t \mapsto \left(t, \frac{d\gamma(t)}{dt}\right)$ belongs to the kernel of the 2-form $d\widehat{\omega}_L$, in other words if and only if*

$$i \left(\frac{d}{dt} \left(t, \frac{d\gamma(t)}{dt} \right) \right) d\widehat{\omega}_L \left(t, \frac{d\gamma(t)}{dt} \right) = 0.$$

The interested reader will find the proof of that theorem in [35], (theorem 2.2, chapter IV, page 262) or, for hyper-regular Lagrangians (an additional assumption which in fact, is not necessary) in [59], chapter IV, theorem 2.1 page 167.

2.4.3 Remark. In his book [55], *Jean-Marie Souriau* uses a slightly different terminology: for him the odd-dimensional space $\mathbb{R} \times TN$ is the *evolution space* of the system, and the exact 2-form $d\widehat{\omega}_L$ on that space is the *Lagrange form*. He defines that 2-form in a setting more general than that of the Lagrangian formalism.

3 Lagrangian symmetries

3.1 Assumptions and notations

In this section N is the configuration space of a conservative Lagrangian mechanical system with a smooth, maybe time dependent Lagrangian $L : \mathbb{R} \times TN \rightarrow \mathbb{R}$. Let $\widehat{\omega}_L$ be the Poincaré-Cartan 1-form on the evolution space $\mathbb{R} \times TN$.

Several kinds of symmetries can be defined for such a system. Very often, they are special cases of *infinitesimal symmetries of the Poincaré-Cartan form*, which play an important part in the famous *Noether theorem*.

3.1.1 Definition. An *infinitesimal symmetry* of the Poincaré-Cartan form $\widehat{\omega}_L$ is a vector field Z on $\mathbb{R} \times TN$ such that

$$\mathcal{L}(Z)\widehat{\omega}_L = 0,$$

$\mathcal{L}(Z)$ denoting the Lie derivative of differential forms with respect to Z .

3.1.2 Examples.

1. Let us assume that the Lagrangian L does not depend on the time $t \in \mathbb{R}$, *i.e.* is a smooth function on TN . The vector field on $\mathbb{R} \times TN$ denoted by $\frac{\partial}{\partial t}$, whose projection on \mathbb{R} is equal to 1 and whose projection on TN is 0, is an infinitesimal symmetry of $\widehat{\omega}_L$.

2. Let X be a smooth vector field on N and \overline{X} be its canonical lift to the tangent bundle TN . We still assume that L does not depend on the time t . Moreover we assume that \overline{X} is an infinitesimal symmetry of the Lagrangian L , *i.e.* that $\mathcal{L}(\overline{X})L = 0$. Considered as a vector field on $\mathbb{R} \times TN$ whose projection on the factor \mathbb{R} is 0, \overline{X} is an infinitesimal symmetry of $\widehat{\omega}_L$.

3.2 The Noether theorem in Lagrangian formalism

3.2.1 Theorem (E. Noether's theorem in Lagrangian formalism). *Let Z be an infinitesimal symmetry of the Poincaré-Cartan form $\widehat{\omega}_L$. For each possible motion $\gamma : [t_0, t_1] \rightarrow N$ of the Lagrangian system, the function $i(Z)\widehat{\omega}_L$, defined on $\mathbb{R} \times TN$, keeps a constant value along the parametrized curve $t \mapsto \left(t, \frac{d\gamma(t)}{dt}\right)$.*

Proof. Let $\gamma : [t_0, t_1] \rightarrow N$ be a motion of the Lagrangian system, *i.e.* a solution of the Euler-Lagrange equations. The Euler-Cartan theorem 2.4.2 proves that, for any $t \in [t_0, t_1]$,

$$i\left(\frac{d}{dt}\left(t, \frac{d\gamma(t)}{dt}\right)\right) d\widehat{\omega}_L\left(t, \frac{d\gamma(t)}{dt}\right) = 0.$$

Since Z is an infinitesimal symmetry of $\widehat{\omega}_L$,

$$\mathcal{L}(Z)\widehat{\omega}_L = 0.$$

Using the well known formula relating the Lie derivative, the interior product and the exterior derivative

$$\mathcal{L}(Z) = i(Z) \circ d + d \circ i(Z)$$

we can write

$$\begin{aligned} \frac{d}{dt} \left(i(Z) \widehat{\omega}_L \left(t, \frac{d\gamma(t)}{dt} \right) \right) &= \left\langle di(Z) \widehat{\omega}_L, \frac{d}{dt} \left(t, \frac{d\gamma(t)}{dt} \right) \right\rangle \\ &= - \left\langle i(Z) d\widehat{\omega}_L, \frac{d}{dt} \left(t, \frac{d\gamma(t)}{dt} \right) \right\rangle \\ &= 0. \end{aligned} \quad \square$$

3.2.2 Example. When the Lagrangian L does not depend on time, application of Emmy Noether's theorem to the vector field $\frac{\partial}{\partial t}$ shows that the energy E_L remains constant during any possible motion of the system, since $i\left(\frac{\partial}{\partial t}\right) \widehat{\omega}_L = -E_L$.

3.2.3 Remarks.

1. Theorem 3.2.1 is due to the German mathematician Emmy Noether (1882–1935), who proved it under much more general assumptions than those used here. For a very nice presentation of Emmy Noether's theorems in a much more general setting and their applications in Mathematical Physics, interested readers are referred to the very nice book by Yvette Kosmann-Schwarzbach [24].

2. Several generalizations of the Noether theorem exist. For example, if instead of being an infinitesimal symmetry of $\widehat{\omega}_L$, *i.e.* instead of satisfying $\mathcal{L}(Z)\widehat{\omega}_L = 0$ the vector field Z satisfies

$$\mathcal{L}(Z)\widehat{\omega}_L = df,$$

where $f : \mathbb{R} \times TM \rightarrow \mathbb{R}$ is a smooth function, which implies of course $\mathcal{L}(Z)(d\widehat{\omega}_L) = 0$, the function

$$i(Z)\widehat{\omega}_L - f$$

keeps a constant value along $t \mapsto \left(t, \frac{d\gamma(t)}{dt} \right)$.

3.3 The Lagrangian momentum map

The Lie bracket of two infinitesimal symmetries of $\widehat{\omega}_L$ is too an infinitesimal symmetry of $\widehat{\omega}_L$. Let us therefore assume that there exists a finite-dimensional Lie algebra of vector fields on $\mathbb{R} \times TN$ whose elements are infinitesimal symmetries of $\widehat{\omega}_L$.

3.3.1 Definition. Let $\psi : \mathcal{G} \rightarrow A^1(\mathbb{R} \times TN)$ be a Lie algebras homomorphism of a finite-dimensional real Lie algebra \mathcal{G} into the Lie algebra of smooth vector fields on $\mathbb{R} \times TN$ such that, for each $X \in \mathcal{G}$, $\psi(X)$ is an infinitesimal symmetry of $\widehat{\omega}_L$. The Lie algebras homomorphism ψ is said to be a *Lie algebra action on $\mathbb{R} \times TN$ by infinitesimal symmetries of $\widehat{\omega}_L$* . The map $K_L : \mathbb{R} \times TN \rightarrow \mathcal{G}^*$, which takes its values in the dual \mathcal{G}^* of the Lie algebra \mathcal{G} , defined by

$$\langle K_L(t, v), X \rangle = i(\psi(X)) \widehat{\omega}_L(t, v), \quad X \in \mathcal{G}, \quad (t, v) \in \mathbb{R} \times TN,$$

is called the *Lagrangian momentum* of the Lie algebra action ψ .

3.3.2 Corollary (of E. Noether's theorem). *Let $\psi : \mathcal{G} \rightarrow A^1(\mathbb{R} \times TM)$ be an action of a finite-dimensional real Lie algebra \mathcal{G} on the evolution space $\mathbb{R} \times TN$ of a conservative Lagrangian system, by infinitesimal symmetries of the Poincaré-Cartan form $\widehat{\omega}_L$. For*

each possible motion $\gamma : [t_0, t_1] \rightarrow N$ of that system, the Lagrangian momentum map K_L keeps a constant value along the parametrized curve $t \mapsto \left(t, \frac{d\gamma(t)}{dt} \right)$.

Proof. Since for each $X \in \mathcal{G}$ the function $(t, v) \mapsto \langle K_L(t, v), X \rangle$ keeps a constant value along the parametrized curve $t \mapsto \left(t, \frac{d\gamma(t)}{dt} \right)$, the map K_L itself keeps a constant value along that parametrized curve. \square

3.3.3 Example. Let us assume that the Lagrangian L does not depend explicitly on the time t and is invariant by the canonical lift to the tangent bundle of the action on N of the six-dimensional group of Euclidean displacements (rotations and translations) of the physical space. The corresponding infinitesimal action of the Lie algebra of infinitesimal Euclidean displacements (considered as an action on $\mathbb{R} \times TN$, the action on the factor \mathbb{R} being trivial) is an action by infinitesimal symmetries of $\widehat{\omega}_L$. The six components of the Lagrangian momentum map are the three components of the total linear momentum and the three components of the total angular momentum.

3.3.4 Remark. These results are valid *without any assumption of hyper-regularity* of the Lagrangian.

3.4 The Euler-Poincaré equation

In a short Note [47] published in 1901, the great french mathematician *Henri Poincaré* (1854–1912) proposed a new formulation of the equations of Mechanics.

Let N be the configuration manifold of a conservative Lagrangian system, with a smooth Lagrangian $L : TN \rightarrow \mathbb{R}$ which does not depend explicitly on time. Poincaré assumes that there exists an homomorphism ψ of a finite-dimensional real Lie algebra \mathcal{G} into the Lie algebra $A^1(N)$ of smooth vector fields on N , such that for each $x \in N$, the values at x of the vector fields $\psi(X)$, when X varies in \mathcal{G} , completely fill the tangent space $T_x N$. The action ψ is then said to be *locally transitive*.

Of course these assumptions imply $\dim \mathcal{G} \geq \dim N$.

Under these assumptions, Henri Poincaré proved that the equations of motion of the Lagrangian system could be written on $N \times \mathcal{G}$ or on $N \times \mathcal{G}^*$, where \mathcal{G}^* is the dual of the Lie algebra \mathcal{G} , instead of on the tangent bundle TN . When $\dim \mathcal{G} = \dim N$ (which can occur only when the tangent bundle TN is trivial) the obtained equation, called the *Euler-Poincaré equation*, is *perfectly equivalent to the Euler-Lagrange equations* and may, in certain cases, be easier to use. But when $\dim \mathcal{G} > \dim N$, the system made by the Euler-Poincaré equation is *underdetermined*.

Let $\gamma : [t_0, t_1] \rightarrow N$ be a smooth parametrized curve in N . Poincaré proves that there exists a smooth curve $V : [t_0, t_1] \rightarrow \mathcal{G}$ in the Lie algebra \mathcal{G} such that, for each $t \in [t_0, t_1]$,

$$\psi(V(t))(\gamma(t)) = \frac{d\gamma(t)}{dt}. \quad (*)$$

When $\dim \mathcal{G} > \dim N$ the smooth curve V in \mathcal{G} is not uniquely determined by the smooth curve γ in N . However, instead of writing the second-order Euler-Lagrange differential equations on TN satisfied by γ when this curve is a possible motion of the Lagrangian system, Poincaré derives a *first order differential equation for the curve V* and proves

that it is satisfied, together with Equation (*), *if and only if* γ is a possible motion of the Lagrangian system.

Let $\varphi : N \times \mathcal{G} \rightarrow TN$ and $\bar{L} : N \times \mathcal{G} \rightarrow \mathbb{R}$ be the maps

$$\varphi(x, X) = \psi(X)(x), \quad \bar{L}(x, X) = L \circ \varphi(x, X).$$

We denote by $d_1\bar{L} : N \times \mathcal{G} \rightarrow T^*N$ and by $d_2\bar{L} : N \times \mathcal{G} \rightarrow \mathcal{G}^*$ the partial differentials of $\bar{L} : N \times \mathcal{G} \rightarrow \mathbb{R}$ with respect to its first variable $x \in N$ and with respect to its second variable $X \in \mathcal{G}$.

The map $\varphi : N \times \mathcal{G} \rightarrow TN$ is a *surjective vector bundles morphism* of the trivial vector bundle $N \times \mathcal{G}$ into the tangent bundle TN . Its *transpose* $\varphi^T : T^*N \rightarrow N \times \mathcal{G}^*$ is therefore an *injective vector bundles morphism*, which can be written

$$\varphi^T(\xi) = (\pi_N(\xi), J(\xi)),$$

where $\pi_N : T^*N \rightarrow N$ is the canonical projection of the cotangent bundle and $J : T^*N \rightarrow \mathcal{G}^*$ is a smooth map whose restriction to each fibre T_x^*N of the cotangent bundle is linear, and is the transpose of the map $X \mapsto \varphi(x, X) = \psi(X)(x)$.

3.4.1 Remark. The homomorphism ψ of the Lie algebra \mathcal{G} into the Lie algebra $A^1(N)$ of smooth vector fields on N is an action of that Lie algebra, in the sense defined below (5.2.1). That action can be canonically lifted into a Hamiltonian action of \mathcal{G} on T^*N , endowed with its canonical symplectic form $d\theta_N$ (5.2.4). The map J is in fact a *Hamiltonian momentum map* for that Hamiltonian action (5.3.1).

Let $\mathcal{L}_L = d_{\text{vert}}L : TN \rightarrow T^*N$ be the *Legendre map* defined in 2.4.1.

3.4.2 Theorem (Euler-Poincaré equation). *With the above defined notations, let $\gamma : [t_0, t_1] \rightarrow N$ be a smooth parametrized curve in N and $V : [t_0, t_1] \rightarrow \mathcal{G}$ be a smooth parametrized curve such that, for each $t \in [t_0, t_1]$,*

$$\psi(V(t))(\gamma(t)) = \frac{d\gamma(t)}{dt}. \quad (*)$$

The curve γ is a possible motion of the Lagrangian system if and only if V satisfies the equation

$$\left(\frac{d}{dt} - \text{ad}_{V(t)}^* \right) \left(J \circ \mathcal{L}_L \circ \varphi(\gamma(t), V(t)) \right) - J \circ d_1\bar{L}(\gamma(t), V(t)) = 0. \quad (**)$$

The interested reader will find a proof of that theorem in local coordinates in the original Note by Poincaré [47]. More intrinsic proofs can be found in [37, 38]. Another proof is possible, in which that theorem is deduced from the Euler-Cartan theorem 2.4.2.

3.4.3 Remark. Equation (*) is called the *compatibility condition* and Equation (**) is the *Euler-Poincaré equation*. It can be written under the equivalent form

$$\left(\frac{d}{dt} - \text{ad}_{V(t)}^* \right) \left(d_2\bar{L}(\gamma(t), V(t)) \right) - J \circ d_1\bar{L}(\gamma(t), V(t)) = 0. \quad (***)$$

Examples of applications of the Euler-Poincaré equation can be found in [18, 37, 38] and, for an application in Thermodynamics, [6].

4 The Hamiltonian formalism

The Lagrangian formalism can be applied to any smooth Lagrangian. Its application yields *second order differential equations* on $\mathbb{R} \times N$ (in local coordinates, the *Euler-Lagrange equations*) which in general *are not solved with respect to the second order derivatives of the unknown functions with respect to time*. The classical existence and unicity theorems for the solutions of differential equations (such as the *Cauchy-Lipschitz theorem*) therefore *cannot be applied to these equations*.

Under the additional assumption that the Lagrangian is *hyper-regular*, a very clever change of variables discovered by *William Rowan Hamilton*² [16, 17] allows a new formulation of these equations in the framework of *symplectic geometry*. The *Hamiltonian formalism* discussed below is the use of these new equations. It was later generalized independently of the Lagrangian formalism.

4.1 Hyper-regular Lagrangians

4.1.1 Assumptions made in this section

We consider in this section a smooth, maybe time-dependent Lagrangian $L : \mathbb{R} \times TN \rightarrow \mathbb{R}$, which is such that the Legendre map (2.4.1) $\mathcal{L}_L : \mathbb{R} \times TN \rightarrow T^*N$ satisfies the following property: for each fixed value of the time $t \in \mathbb{R}$, the map $v \mapsto \mathcal{L}_L(t, v)$ is a smooth diffeomorphism of the tangent bundle TN onto the cotangent bundle T^*N . An equivalent assumption is the following: the map $(\text{id}_{\mathbb{R}}, \mathcal{L}_L) : (t, v) \mapsto (t, \mathcal{L}_L(t, v))$ is a smooth diffeomorphism of $\mathbb{R} \times TN$ onto $\mathbb{R} \times T^*N$. The Lagrangian L is then said to be *hyper-regular*. The equations of motion can be written on $\mathbb{R} \times T^*N$ instead of $\mathbb{R} \times TN$.

4.1.2 Definitions. Under the assumption 4.1.1, the function $H_L : \mathbb{R} \times T^*N \rightarrow \mathbb{R}$ given by

$$H_L(t, p) = E_L \circ (\text{id}_{\mathbb{R}}, \mathcal{L}_L)^{-1}(t, p), \quad t \in \mathbb{R}, p \in T^*N,$$

($E_L : \mathbb{R} \times TN \rightarrow \mathbb{R}$ being the *energy function* defined in 2.4.1) is called the *Hamiltonian* associated to the hyper-regular Lagrangian L .

The 1-form defined on $\mathbb{R} \times T^*N$

$$\widehat{\omega}_{H_L} = \theta_N - H_L dt,$$

where θ_N is the *Liouville 1-form* on T^*N , is called the *Poincaré-Cartan 1-form in the Hamiltonian formalism*.

4.1.3 Remark. The *Poincaré-Cartan 1-form* $\widehat{\omega}_L$ on $\mathbb{R} \times TN$, defined in 2.4.1, is the pull-back, by the diffeomorphism $(\text{id}_{\mathbb{R}}, \mathcal{L}_L) : \mathbb{R} \times TN \rightarrow \mathbb{R} \times T^*N$, of the Poincaré-Cartan 1-form $\widehat{\omega}_{H_L}$ in the Hamiltonian formalism on $\mathbb{R} \times T^*N$ defined above.

4.2 Presymplectic manifolds

4.2.1 Definitions. A *presymplectic form* on a smooth manifold M is a 2-form ω on M which is closed, *i.e.* such that $d\omega = 0$. A manifold M equipped with a presymplectic form ω is called a *presymplectic manifold* and denoted by (M, ω) .

The *kernel* $\ker \omega$ of a presymplectic form ω defined on a smooth manifold M is the set of vectors $v \in TM$ such that $i(v)\omega = 0$.

²*Lagrange* obtained however *Hamilton's equations* before *Hamilton*, but only in a special case, for the slow “variations of constants” such as the orbital parameters of planets in the solar system [26, 27].

4.2.2 Remarks. A symplectic form ω on a manifold M is a presymplectic form which, moreover, is non-degenerate, *i.e.* such that for each $x \in M$ and each non-zero vector $v \in T_x M$, there exists another vector $w \in T_x M$ such that $\omega(x)(v, w) \neq 0$. Or in other words, a presymplectic form ω whose kernel is the set of null vectors.

The kernel of a presymplectic form ω on a smooth manifold M is a vector sub-bundle of TM if and only if for each $x \in M$, the vector subspace $T_x M$ of vectors $v \in T_x M$ which satisfy $i(v)\omega = 0$ is of a fixed dimension, the same for all points $x \in M$. A presymplectic form which satisfies that condition is said to be of *constant rank*.

4.2.3 Proposition. *Let ω be a presymplectic form of constant rank (4.2.2) on a smooth manifold M . The kernel $\ker \omega$ of ω is a completely integrable vector sub-bundle of TM , which defines a foliation \mathcal{F}_ω of M into connected immersed submanifolds which, at each point of M , have the fibre of $\ker \omega$ at that point as tangent vector space.*

We now assume in addition that this foliation is simple, i.e. such that the set of leaves of \mathcal{F}_ω , denoted by $M/\ker \omega$, has a smooth manifold structure for which the canonical projection $p : M \rightarrow M/\ker \omega$ (which associates to each point $x \in M$ the leaf which contains x) is a smooth submersion. There exists on $M/\ker \omega$ a unique symplectic form ω_r such that

$$\omega = p^* \omega_r.$$

Proof. Since $d\omega = 0$, the fact that $\ker \omega$ is completely integrable is an immediate consequence of the Frobenius' theorem ([59], chapter III, theorem 5.1 page 132). The existence and unicity of a symplectic form ω_r on $M/\ker \omega$ such that $\omega = p^* \omega_r$ results from the fact that $M/\ker \omega$ is built by quotienting M by the kernel of ω . \square

4.2.4 Presymplectic manifolds in Mechanics

Let us go back to the assumptions and notations of 4.1.1. We have seen in 4.1.3 that the Poincaré-Cartan 1-form in Hamiltonian formalism $\widehat{\omega}_{H_L}$ on $\mathbb{R} \times T^*N$ and the Poincaré-Cartan 1-form in Lagrangian formalism $\widehat{\omega}_L$ on $\mathbb{R} \times TN$ are related by

$$\widehat{\omega}_L = (\text{id}_{\mathbb{R}}, \mathcal{L}_L)^* \widehat{\omega}_{H_L}.$$

Their exterior differentials $d\widehat{\omega}_L$ and $d\widehat{\omega}_{H_L}$ both are *presymplectic 2-forms* on the odd-dimensional manifolds $\mathbb{R} \times TN$ and $\mathbb{R} \times T^*N$, respectively. At any point of these manifolds, the kernels of these closed 2 forms are one-dimensional. They therefore (4.2.3) determine *foliations into smooth curves* of these manifolds. The Euler-Cartan theorem (2.4.2) shows that each of these curves is a possible *motion* of the system, described either in the Lagrangian formalism, or in the Hamiltonian formalism, respectively.

The set of all possible motions of the system, called by Jean-Marie Souriau the *manifold of motions* of the system, is described by the quotient $(\mathbb{R} \times TN)/\ker d\widehat{\omega}_L$ in the Lagrangian formalism, and by the quotient $(\mathbb{R} \times T^*N)/\ker d\widehat{\omega}_{H_L}$ in the Hamiltonian formalism. Both are (maybe non-Hausdorff) *symplectic manifolds*, the projections on these quotient manifolds of the presymplectic forms $d\widehat{\omega}_L$ and $d\widehat{\omega}_{H_L}$ both being symplectic forms. Of course the diffeomorphism $(\text{id}_{\mathbb{R}}, \mathcal{L}_L) : \mathbb{R} \times TN \rightarrow \mathbb{R} \times T^*N$ projects onto a symplectomorphism between the Lagrangian and Hamiltonian descriptions of the manifold of motions of the system.

4.3 The Hamilton equation

4.3.1 Proposition. *Let N be the configuration manifold of a Lagrangian system whose Lagrangian $L : \mathbb{R} \times TN \rightarrow \mathbb{R}$, maybe time-dependent, is smooth and hyper-regular, and $H_L : \mathbb{R} \times T^*N \rightarrow \mathbb{R}$ be the associated Hamiltonian (4.1.2). Let $\varphi : [t_0, t_1] \rightarrow N$ be a smooth curve parametrized by the time $t \in [t_0, t_1]$, and let $\psi : [t_0, t_1] \rightarrow T^*N$ be the parametrized curve in T^*N*

$$\psi(t) = \mathcal{L}_L \left(t, \frac{d\gamma(t)}{dt} \right), \quad t \in [t_0, t_1],$$

where $\mathcal{L}_L : \mathbb{R} \times TN \rightarrow T^*N$ is the Legendre map (2.4.1).

The parametrized curve $t \mapsto \gamma(t)$ is a motion of the system if and only if the parametrized curve $t \mapsto \psi(t)$ satisfies the equation, called the Hamilton equation,

$$i \left(\frac{d\psi(t)}{dt} \right) d\theta_N = -dH_{L_t},$$

where $dH_{L_t} = dH_L - \frac{\partial H_L}{\partial t} dt$ is the differential of the function $H_{L_t} : T^*N \rightarrow \mathbb{R}$ in which the time t is considered as a parameter with respect to which there is no differentiation.

When the parametrized curve ψ satisfies the Hamilton equation stated above, it satisfies too the equation, called the energy equation

$$\frac{d}{dt} \left(H_L(t, \psi(t)) \right) = \frac{\partial H_L}{\partial t} (t, \psi(t)).$$

Proof. These results directly follow from the Euler-Cartan theorem (2.4.2). \square

4.3.2 Remarks. The 2-form $d\theta_N$ is a symplectic form on the cotangent bundle T^*N , called its *canonical symplectic form*. We have shown that when the Lagrangian L is hyper-regular, the equations of motion can be written in *three equivalent manners*:

1. as the *Euler-Lagrange equations* on $\mathbb{R} \times TM$,
2. as the equations given by the *kernels of the presymplectic forms* $d\widehat{\omega}_L$ or $d\widehat{\omega}_{H_L}$ which determine the foliations into curves of the evolution spaces $\mathbb{R} \times TM$ in the Lagrangian formalism, or $\mathbb{R} \times T^*M$ in the Hamiltonian formalism,
3. as the *Hamilton equation* associated to the Hamiltonian H_L on the symplectic manifold $(T^*N, d\theta_N)$, often called the *phase space* of the system.

4.3.3 The Tulczyjew isomorphisms

Around 1974, *W.M. Tulczyjew* [61, 62] discovered ³ two remarkable vector bundles isomorphisms $\alpha_N : TT^*N \rightarrow T^*TN$ and $\beta_N : TT^*N \rightarrow T^*T^*N$.

The first one α_N is an isomorphism of the bundle $(TT^*N, T\pi_N, TN)$ onto the bundle (T^*TN, π_{TN}, TN) , while the second β_N is an isomorphism of the bundle $(TT^*N, \tau_{T^*N}, T^*N)$

³ β_N was probably known long before 1974, but I believe that α_N , much more hidden, was noticed by Tulczyjew for the first time.

onto the bundle $(T^*T^*N, \pi_{T^*N}, T^*N)$. The diagram below is commutative.

$$\begin{array}{ccccc}
T^*T^*N & \xleftarrow{\beta_N} & TT^*N & \xrightarrow{\alpha_N} & T^*TN \\
\pi_{T^*N} \downarrow & & \swarrow \tau_{T^*N} & & \searrow T\pi_N \\
T^*N & & & & TN \\
& \searrow \pi_N & & & \swarrow \tau_N \\
& & N & &
\end{array}$$

Since they are the total spaces of cotangent bundles, the manifolds T^*TN and T^*T^*N are endowed with the Liouville 1-forms θ_{TN} and θ_{T^*N} , and with the canonical symplectic forms $d\theta_{TN}$ and $d\theta_{T^*N}$, respectively. Using the isomorphisms α_N and β_N , we can therefore define on TT^*N two 1-forms $\alpha_N^*\theta_{TN}$ and $\beta_N^*\theta_{T^*N}$, and two symplectic 2-forms $\alpha_N^*(d\theta_{TN})$ and $\beta_N^*(d\theta_{T^*N})$. The very remarkable property of the isomorphisms α_N and β_N is that *the two symplectic forms so obtained on TT^*N are equal*:

$$\alpha_N^*(d\theta_{TN}) = \beta_N^*(d\theta_{T^*N}).$$

The 1-forms $\alpha_N^*\theta_{TN}$ and $\beta_N^*\theta_{T^*N}$ are not equal, their difference is the differential of a smooth function.

4.3.4 Lagrangian submanifolds

In view of applications to implicit Hamiltonian systems, let us recall here that a Lagrangian submanifold of a symplectic manifold (M, ω) is a submanifold N whose dimension is half the dimension of M , on which the form induced by the symplectic form ω is 0.

Let $L : TN \rightarrow \mathbb{R}$ and $H : T^*N \rightarrow \mathbb{R}$ be two smooth real valued functions, defined on TN and on T^*N , respectively. The graphs $dL(TN)$ and $dH(T^*N)$ of their differentials are Lagrangian submanifolds of the symplectic manifolds $(T^*TN, d\theta_{TN})$ and $(T^*T^*N, d\theta_{T^*N})$. Their pull-backs $\alpha_N^{-1}(dL(TN))$ and $\beta_N^{-1}(dH(T^*N))$ by the symplectomorphisms α_N and β_N are therefore two Lagrangian submanifolds of the manifold TT^*N endowed with the symplectic form $\alpha_N^*(d\theta_{TN})$, which is equal to the symplectic form $\beta_N^*(d\theta_{T^*N})$.

The following theorem enlightens some aspects of the relationships between the Hamiltonian and the Lagrangian formalisms.

4.3.5 Theorem (W.M. Tulczyjew). *With the notations specified above (4.3.4), let $X_H : T^*N \rightarrow TT^*N$ be the Hamiltonian vector field on the symplectic manifold $(T^*N, d\theta_N)$ associated to the Hamiltonian $H : T^*N \rightarrow \mathbb{R}$, defined by $i(X_H)d\theta_N = -dH$. Then*

$$X_H(T^*N) = \beta_N^{-1}(dH(T^*N)).$$

Moreover, the equality

$$\alpha_N^{-1}(dL(TN)) = \beta_N^{-1}(dH(T^*N))$$

holds if and only if the Lagrangian L is hyper-regular and such that

$$dH = d(E_L \circ \mathcal{L}_L^{-1}),$$

where $\mathcal{L}_L : TN \rightarrow T^*N$ is the Legendre map and $E_L : TN \rightarrow \mathbb{R}$ the energy associated to the Lagrangian L .

The interested reader will find the proof of that theorem in the works of W. Tulczyjew ([61, 62]).

When L is not hyper-regular, $\alpha_N^{-1}(dL(TN))$ still is a Lagrangian submanifold of the symplectic manifold $(TT^*N, \alpha_N^*(d\theta_{TN}))$, but it is no more the graph of a smooth vector field X_H defined on T^*N . Tulczyjew proposes to consider this Lagrangian submanifold as an *implicit Hamilton equation* on T^*N .

These results can be extended to Lagrangians and Hamiltonians which may depend on time.

4.4 The Hamiltonian formalism on symplectic and Poisson manifolds

4.4.1 The Hamilton formalism on symplectic manifolds

In pure mathematics as well as in applications of mathematics to Mechanics and Physics, symplectic manifolds other than cotangent bundles are encountered. A theorem due to the french mathematician *Gaston Darboux* (1842–1917) asserts that any symplectic manifold (M, ω) is of even dimension $2n$ and is locally isomorphic to the cotangent bundle to a n -dimensional manifold: in a neighbourhood of each of its point there exist local coordinates $(x^1, \dots, x^n, p_1, \dots, p_n)$, called *Darboux coordinates* with which the symplectic form ω is expressed exactly as the canonical symplectic form of a cotangent bundle:

$$\omega = \sum_{i=1}^n dp_i \wedge dx^i.$$

Let (M, ω) be a symplectic manifold and $H : \mathbb{R} \times M \rightarrow \mathbb{R}$ a smooth function, said to be a *time-dependent Hamiltonian*. It determines a *time-dependent Hamiltonian vector field* X_H on M , such that

$$i(X_H)\omega = -dH_t,$$

$H_t : M \rightarrow \mathbb{R}$ being the function H in which the variable t is considered as a parameter with respect to which no differentiation is made.

The *Hamilton equation* determined by H is the differential equation

$$\frac{d\psi(t)}{dt} = X_H(t, \psi(t)).$$

The Hamiltonian formalism can therefore be applied to any smooth, maybe time dependent Hamiltonian on M , even when there is no associated Lagrangian.

The Hamiltonian formalism is not limited to symplectic manifolds: it can be applied, for example, to *Poisson manifolds* [32], *contact manifolds* and *Jacobi manifolds* [33]. For simplicity I will consider only Poisson manifolds. Readers interested in Jacobi manifolds and their generalizations are referred to the papers by A. Lichnerowicz quoted above and to the very important paper by A. Kirillov [23].

4.4.2 Definition. A *Poisson manifold* is a smooth manifold P whose algebra of smooth functions $C^\infty(P, \mathbb{R})$ is endowed with a bilinear composition law, called the *Poisson bracket*, which associates to any pair (f, g) of smooth functions on P another smooth function denoted by $\{f, g\}$, that composition satisfying the three properties

1. it is skew-symmetric,

$$\{g, f\} = -\{f, g\},$$

2. it satisfies the *Jacobi identity*

$$\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0,$$

3. it satisfies the *Leibniz identity*

$$\{f, gh\} = \{f, g\}h + g\{f, h\}.$$

4.4.3 Examples.

1. On the vector space of smooth functions defined on a symplectic manifold (M, ω) , there exists a composition law, called the *Poisson bracket*, which satisfies the properties stated in 4.4.2. Let us recall briefly its definition. The symplectic form ω allows us to associate, to any smooth function $f \in C^\infty(M, \mathbb{R})$, a smooth vector field $X_f \in A^1(M, \mathbb{R})$, called the *Hamiltonian vector field associated to f* , defined by

$$i(X_f)\omega = -df.$$

The Poisson bracket $\{f, g\}$ of two smooth functions f and $g \in C^\infty(M, \mathbb{R})$ is defined by the three equivalent equalities

$$\{f, g\} = i(X_f)dg = -i(X_g)df = \omega(X_f, X_g).$$

Any symplectic manifold is therefore a Poisson manifold.

The Poisson bracket of smooth functions defined on a symplectic manifold (when that symplectic manifold is a cotangent bundle) was discovered by Siméon Denis Poisson (1781–1840) [48].

2. Let \mathcal{G} be a finite-dimensional real Lie algebra, and let \mathcal{G}^* be its dual vector space. For each smooth function $f \in C^\infty(\mathcal{G}^*, \mathbb{R})$ and each $\zeta \in \mathcal{G}^*$, the differential $df(\zeta)$ is a linear form on \mathcal{G}^* , in other words an element of the dual vector space of \mathcal{G}^* . Identifying with \mathcal{G} the dual vector space of \mathcal{G}^* , we can therefore consider $df(\zeta)$ as an element in \mathcal{G} . With this identification, we can define the Poisson bracket of two smooth functions f and $g \in C^\infty(\mathcal{G}^*, \mathbb{R})$ by

$$\{f, g\}(\zeta) = [df(\zeta), dg(\zeta)], \quad \zeta \in \mathcal{G}^*,$$

the bracket in the right hand side being the bracket in the Lie algebra \mathcal{G} . The Poisson bracket of functions in $C^\infty(\mathcal{G}^*, \mathbb{R})$ so defined satisfies the properties stated in 4.4.2. The dual vector space of any finite-dimensional real Lie algebra is therefore endowed with a Poisson structure, called its *canonical Lie-Poisson structure* or its *Kirillov-Kostant-Souriau Poisson structure*. Discovered by Sophus Lie, this structure was indeed rediscovered independently by Alexander Kirillov, Bertram Kostant and Jean-Marie Souriau.

3. A *symplectic cocycle* of a finite-dimensional, real Lie algebra \mathcal{G} is a skew-symmetric bilinear map $\Theta : \mathcal{G} \times \mathcal{G} \rightarrow \mathcal{G}^*$ which satisfies, for all X, Y and $Z \in \mathcal{G}$,

$$\Theta([X, Y], Z) + \Theta([Y, Z], X) + \Theta([Z, X], Y) = 0.$$

The canonical Lie-Poisson bracket of two smooth functions f and $g \in C^\infty(\mathcal{G}^*, \mathbb{R})$ can be modified by means of the symplectic cocycle Θ , by setting

$$\{f, g\}_\Theta(\zeta) = [df(\zeta), dg(\zeta)] - \Theta(df(\zeta), dg(\zeta)), \quad \zeta \in \mathcal{G}^*.$$

This bracket still satisfies the properties stated in 4.4.2, therefore defines on \mathcal{G}^* a Poisson structure called its *canonical Lie-Poisson structure modified by Θ* .

4.4.4 Properties of Poisson manifolds

The interested reader will find the proofs of the properties recalled here in [63], [31], [30] or [45].

1. On a Poisson manifold P , the Poisson bracket $\{f, g\}$ of two smooth functions f and g can be expressed by means of a smooth field of bivectors Λ :

$$\{f, g\} = \Lambda(df, dg), \quad f \text{ and } g \in C^\infty(P, \mathbb{R}),$$

called the *Poisson bivector field* of P . The considered Poisson manifold is often denoted by (P, Λ) . The Poisson bivector field Λ identically satisfies

$$[\Lambda, \Lambda] = 0,$$

the bracket $[\ , \]$ in the left hand side being the *Schouten-Nijenhuis bracket*. That bivector field determines a vector bundle morphism $\Lambda^\sharp : T^*P \rightarrow TP$, defined by

$$\Lambda(\eta, \zeta) = \langle \zeta, \Lambda^\sharp(\eta) \rangle,$$

where η and $\zeta \in T^*P$ are two covectors attached to the same point in P .

Readers interested in the Schouten-Nijenhuis bracket will find thorough presentations of its properties in [25] or [36].

2. Let (P, Λ) be a Poisson manifold. A (maybe time-dependent) vector field on P can be associated to each (maybe time-dependent) smooth function $H : \mathbb{R} \times P \rightarrow \mathbb{R}$. It is called the *Hamiltonian vector field* associated to the *Hamiltonian* H , and denoted by X_H . Its expression is

$$X_H(t, x) = \Lambda^\sharp(x)(dH_t(x)),$$

where $dH_t(x) = dH(t, x) - \frac{\partial H(t, x)}{\partial t} dt$ is the differential of the function deduced from H by considering t as a parameter with respect to which no differentiation is made.

The *Hamilton equation* determined by the (maybe time-dependent) Hamiltonian H is

$$\frac{d\varphi(t)}{dt} = X_H((t, \varphi(t))) = \Lambda^\sharp(dH_t)(\varphi(t)).$$

3. Any Poisson manifold is foliated, by a generalized foliation whose leaves may not be all of the same dimension, into immersed connected symplectic manifolds called the *symplectic leaves* of the Poisson manifold. The value, at any point of a Poisson manifold, of the Poisson bracket of two smooth functions only depends on the restrictions of these functions to the symplectic leaf through the considered point, and can be calculated as the Poisson bracket of functions defined on that leaf, with the Poisson structure associated to the symplectic structure of that leaf. This property was discovered by Alan Weinstein, in his very thorough study of the local structure of Poisson manifolds [64].

5 Hamiltonian symmetries

5.1 Presymplectic, symplectic and Poisson maps and vector fields

Let M be a manifold endowed with some structure, which can be either

- a *presymplectic structure*, determined by a presymplectic form, *i.e.*, a 2-form ω which is closed ($d\omega = 0$),
- a *symplectic structure*, determined by a symplectic form ω , *i.e.*, a 2-form ω which is both closed ($d\omega = 0$) and nondegenerate ($\ker \omega = \{0\}$),
- a *Poisson structure*, determined by a smooth Poisson bivector field Λ satisfying $[\Lambda, \Lambda] = 0$.

5.1.1 Definition. A *presymplectic* (resp. *symplectic*, resp. *Poisson*) diffeomorphism of a presymplectic (resp., symplectic, resp. Poisson) manifold (M, ω) (resp. (M, Λ)) is a smooth diffeomorphism $f : M \rightarrow M$ such that $f^*\omega = \omega$ (resp. $f^*\Lambda = \Lambda$).

5.1.2 Definition. A smooth vector field X on a presymplectic (resp. symplectic, resp. Poisson) manifold (M, ω) (resp. (M, Λ)) is said to be a *presymplectic* (resp. *symplectic*, resp. *Poisson*) vector field if $\mathcal{L}(X)\omega = 0$ (resp. if $\mathcal{L}(X)\Lambda = 0$), where $\mathcal{L}(X)$ denotes the Lie derivative of forms or multivector fields with respect to X .

5.1.3 Definition. Let (M, ω) be a presymplectic or symplectic manifold. A smooth vector field X on M is said to be *Hamiltonian* if there exists a smooth function $H : M \rightarrow \mathbb{R}$, called a *Hamiltonian* for X , such that

$$i(X)\omega = -dH.$$

Not any smooth function on a presymplectic manifold can be a Hamiltonian.

5.1.4 Definition. Let (M, Λ) be a Poisson manifold. A smooth vector field X on M is said to be *Hamiltonian* if there exists a smooth function $H \in C^\infty(M, \mathbb{R})$, called a *Hamiltonian* for X , such that $X = \Lambda^\sharp(dH)$. An equivalent definition is that

$$i(X)dg = \{H, g\} \quad \text{for any } g \in C^\infty(M, \mathbb{R}),$$

where $\{H, g\} = \Lambda(dH, dg)$ denotes the Poisson bracket of the functions H and g .

On a symplectic or a Poisson manifold, any smooth function can be a Hamiltonian.

5.1.5 Proposition. A *Hamiltonian vector field* on a *presymplectic* (resp. *symplectic*, resp. *Poisson*) manifold automatically is a *presymplectic* (resp. *symplectic*, resp. *Poisson*) vector field.

The proof of this result, which is easy, can be found in any book on symplectic and Poisson geometry, for example [31], [30] or [45].

5.2 Lie algebras and Lie groups actions

5.2.1 Definitions. An *action on the left* (resp. an *action on the right*) of a Lie group G on a smooth manifold M is a smooth map $\Phi : G \times M \rightarrow M$ (resp. a smooth map $\Psi : M \times G \rightarrow M$) such that

- for each fixed $g \in G$, the map $\Phi_g : M \rightarrow M$ defined by $\Phi_g(x) = \Phi(g, x)$ (resp. the map $\Psi_g : M \rightarrow M$ defined by $\Psi_g(x) = \Psi(x, g)$) is a smooth diffeomorphism of M ,
- $\Phi_e = \text{id}_M$ (resp. $\Psi_e = \text{id}_M$), e being the neutral element of G ,
- for each pair $(g_1, g_2) \in G \times G$, $\Phi_{g_1} \circ \Phi_{g_2} = \Phi_{g_1 g_2}$ (resp. $\Psi_{g_1} \circ \Psi_{g_2} = \Psi_{g_2 g_1}$).

An *action* of a Lie algebra \mathfrak{G} on a smooth manifold M is a *Lie algebras morphism* of \mathfrak{G} into the Lie algebra $A^1(M)$ of smooth vector fields on M , i.e. a linear map $\psi : \mathfrak{G} \rightarrow A^1(M)$ which associates to each $X \in \mathfrak{G}$ a smooth vector field $\psi(X)$ on M such that for each pair $(X, Y) \in \mathfrak{G} \times \mathfrak{G}$, $\psi([X, Y]) = [\psi(X), \psi(Y)]$.

5.2.2 Proposition. *An action Ψ , either on the left or on the right, of a Lie group G on a smooth manifold M , automatically determines an action ψ of its Lie algebra \mathfrak{G} on that manifold, which associates to each $X \in \mathfrak{G}$ the vector field $\psi(X)$ on M , often denoted by X_M and called the *fundamental vector field* on M associated to X . It is defined by*

$$\psi(X)(x) = X_M(x) = \left. \frac{d}{ds} (\Psi_{\exp(sX)}(x)) \right|_{s=0}, \quad x \in M,$$

with the following convention: ψ is a Lie algebras homomorphism when we take for Lie algebra \mathfrak{G} of the Lie group G the Lie algebra or right invariant vector fields on G if Ψ is an action on the left, and the Lie algebra of left invariant vector fields on G if Ψ is an action on the right.

Proof. If Ψ is an action of G on M on the left (respectively, on the right), the vector field on G which is right invariant (respectively, left invariant) and whose value at e is X , and the associated fundamental vector field X_M on M , are compatible by the map $g \mapsto \Psi_g(x)$. Therefore the map $\psi : \mathfrak{G} \rightarrow A^1(M)$ is a Lie algebras homomorphism, if we take for definition of the bracket on \mathfrak{G} the bracket of right invariant (respectively, left invariant) vector fields on G . \square

5.2.3 Definitions. When M is a presymplectic (or a symplectic, or a Poisson) manifold, an action Ψ of a Lie group G (respectively, an action ψ of a Lie algebra \mathfrak{G}) on the manifold M is called a presymplectic (or a symplectic, or a Poisson) action if for each $g \in G$, Ψ_g is a presymplectic, or a symplectic, or a Poisson diffeomorphism of M (respectively, if for each $X \in \mathfrak{G}$, $\psi(X)$ is a presymplectic, or a symplectic, or a Poisson vector field on M).

5.2.4 Definitions. An action ψ of a Lie algebra \mathfrak{G} on a presymplectic or symplectic manifold (M, ω) , or on a Poisson manifold (M, Λ) , is said to be *Hamiltonian* if for each $X \in \mathfrak{G}$, the vector field $\psi(X)$ on M is Hamiltonian.

An action Ψ (either on the left or on the right) of a Lie group G on a presymplectic or symplectic manifold (M, ω) , or on a Poisson manifold (M, Λ) , is said to be *Hamiltonian* if that action is presymplectic, or symplectic, or Poisson (according to the structure of M), and if in addition the associated action of the Lie algebra \mathfrak{G} of G is Hamiltonian.

5.2.5 Remark. A Hamiltonian action of a Lie group, or of a Lie algebra, on a presymplectic, symplectic or Poisson manifold, is automatically a presymplectic, symplectic or Poisson action. This result immediately follows from [5.1.5](#)

5.3 Momentum maps of Hamiltonian actions

5.3.1 Proposition. *Let ψ be a Hamiltonian action of a finite-dimensional Lie algebra \mathfrak{G} on a presymplectic, symplectic or Poisson manifold (M, ω) or (M, Λ) . There exists a smooth map $J : M \rightarrow \mathfrak{G}^*$, taking its values in the dual space \mathfrak{G}^* of the Lie algebra \mathfrak{G} , such that for each $X \in \mathfrak{G}$ the Hamiltonian vector field $\psi(X)$ on M admits as Hamiltonian the function $J_X : M \rightarrow \mathbb{R}$, defined by*

$$J_X(x) = \langle J(x), X \rangle, \quad x \in M.$$

The map J is called a momentum map for the Lie algebra action ψ . When ψ is the action of the Lie algebra \mathfrak{G} of a Lie group G associated to a Hamiltonian action Ψ of a Lie group G , J is called a momentum map for the Hamiltonian Lie group action Ψ .

The proof of that result, which is easy, can be found for example in [31], [30] or [45].

5.3.2 Remark. The momentum map J is not unique:

- when (M, ω) is a connected symplectic manifold, J is determined up to addition of an arbitrary constant element in \mathfrak{G}^* ;
- when (M, Λ) is a connected Poisson manifold, the momentum map J is determined up to addition of an arbitrary \mathfrak{G}^* -valued smooth map which, coupled with any $X \in \mathfrak{G}$, yields a Casimir of the Poisson algebra of (M, Λ) , i.e. a smooth function on M whose Poisson bracket with any other smooth function on that manifold is the function identically equal to 0.

5.4 Noether's theorem in Hamiltonian formalism

5.4.1 Theorem (Noether's theorem in Hamiltonian formalism). *Let X_f and X_g be two Hamiltonian vector fields on a presymplectic or symplectic manifold (M, ω) , or on a Poisson manifold (M, Λ) , which admit as Hamiltonians, respectively, the smooth functions f and g on the manifold M . The function f remains constant on each integral curve of X_g if and only if g remains constant on each integral curve of X_f .*

Proof. The function f is constant on each integral curve of X_g if and only if $i(X_g)df = 0$, since each integral curve of X_g is connected. We can use the Poisson bracket, even when M is a presymplectic manifold, since the Poisson bracket of two Hamiltonians on a presymplectic manifold still can be defined. So we can write

$$i(X_g)df = \{g, f\} = -\{f, g\} = -i(X_f)dg. \quad \square$$

5.4.2 Corollary (of Noether's theorem in Hamiltonian formalism). *Let $\psi : \mathfrak{G} \rightarrow A^1(M)$ be a Hamiltonian action of a finite-dimensional Lie algebra \mathfrak{G} on a presymplectic or symplectic manifold (M, ω) , or on a Poisson manifold (M, Λ) , and let $J : M \rightarrow \mathfrak{G}^*$ be a momentum map of this action. Let X_H be a Hamiltonian vector field on M admitting as Hamiltonian a smooth function H . If for each $X \in \mathfrak{G}$ we have $i(\psi(X))(dH) = 0$, the momentum map J remains constant on each integral curve of X_H .*

Proof. This result is obtained by applying 5.4.1 to the pairs of Hamiltonian vector fields made by X_H and each vector field associated to an element of a basis of \mathfrak{G} . \square

5.5 Symplectic cocycles

5.5.1 Theorem (J.M. Souriau). *Let Φ be a Hamiltonian action (either on the left or on the right) of a Lie group G on a connected symplectic manifold (M, ω) and let $J : M \rightarrow \mathfrak{G}^*$ be a momentum map of this action. There exists an affine action A (either on the left or on the right) of the Lie group G on the dual \mathfrak{G}^* of its Lie algebra \mathfrak{G} such that the momentum map J is equivariant with respect to the actions Φ of G on M and A of G on \mathfrak{G}^* , i.e. such that*

$$J \circ \Phi_g(x) = A_g \circ J(x) \quad \text{for all } g \in G, x \in M.$$

The action A can be written, with $g \in G$ and $\xi \in \mathfrak{G}^*$,

$$\begin{cases} A(g, \xi) = \text{Ad}_{g^{-1}}^*(\xi) + \theta(g) & \text{if } \Phi \text{ is an action on the left,} \\ A(\xi, g) = \text{Ad}_g^*(\xi) - \theta(g^{-1}) & \text{if } \Phi \text{ is an action on the right.} \end{cases}$$

Proof. Let us assume that Φ is an action on the left. The fundamental vector field X_M associated to each $X \in \mathfrak{G}$ is Hamiltonian, with the function $J_X : M \rightarrow \mathbb{R}$, given by

$$J_X(x) = \langle J(x), X \rangle, \quad x \in M,$$

as Hamiltonian. For each $g \in G$ the direct image $(\Phi_{g^{-1}})_*(X_M)$ of X_M by the symplectic diffeomorphism $\Phi_{g^{-1}}$ is Hamiltonian, with $J_X \circ \Phi_g$ as Hamiltonian. An easy calculation shows that this vector field is the fundamental vector field associated to $\text{Ad}_{g^{-1}}(X) \in \mathfrak{G}$. The function

$$x \mapsto \langle J(x), \text{Ad}_{g^{-1}}(X) \rangle = \langle \text{Ad}_{g^{-1}}^* \circ J(x), X \rangle$$

is therefore a Hamiltonian for that vector field. These two functions defined on the connected manifold M , which both are admissible Hamiltonians for the same Hamiltonian vector field, differ only by a constant (which may depend on $g \in G$). We can set, for any $g \in G$,

$$\theta(g) = J \circ \Phi_g(x) - \text{Ad}_{g^{-1}}^* \circ J(x)$$

and check that the map $A : G \times \mathfrak{G}^* \rightarrow \mathfrak{G}^*$ defined in the statement is indeed an action for which J is equivariant.

A similar proof, with some changes of signs, holds when Φ is an action on the right. \square

5.5.2 Proposition. *Under the assumptions and with the notations of 5.5.1, the map $\theta : G \rightarrow \mathfrak{G}^*$ is a cocycle of the Lie group G with values in \mathfrak{G}^* , for the coadjoint representation. It means that it satisfies, for all g and $h \in G$,*

$$\theta(gh) = \theta(g) + \text{Ad}_{g^{-1}}^*(\theta(h)).$$

More precisely θ is a symplectic cocycle. It means that its differential $T_e\theta : T_eG \cong \mathfrak{G} \rightarrow \mathfrak{G}^$ at the neutral element $e \in G$ can be considered as a skew-symmetric bilinear form on \mathfrak{G} :*

$$\Theta(X, Y) = \langle T_e\theta(X), Y \rangle = -\langle T_e\theta(Y), X \rangle.$$

The skew-symmetric bilinear form Θ is a symplectic cocycle of the Lie algebra \mathfrak{G} . It means that it is skew-symmetric and satisfies, for all X, Y and $Z \in \mathfrak{G}$,

$$\Theta([X, Y], Z) + \Theta([Y, Z], X) + \Theta([Z, X], Y) = 0.$$

Proof. These properties easily follow from the fact that when Φ is an action on the left, for g and $h \in G$, $\Phi_g \circ \Phi_h = \Phi_{gh}$ (and a similar equality when Φ is an action on the right). The interested reader will find more details in [31], [55] or [38]. \square

5.5.3 Proposition. *Still under the assumptions and with the notations of 5.5.1, the composition law which associates to each pair (f, g) of smooth real-valued functions on \mathfrak{G}^* the function $\{f, g\}_\Theta$ given by*

$$\{f, g\}_\Theta(x) = \langle x, [df(x), dg(x)] \rangle - \Theta(df(x), dg(x)), \quad x \in \mathfrak{G}^*,$$

*(\mathfrak{G} being identified with its bidual \mathfrak{G}^{**}), determines a Poisson structure on \mathfrak{G}^* , and the momentum map $J : M \rightarrow \mathfrak{G}^*$ is a Poisson map, M being endowed with the Poisson structure associated to its symplectic structure.*

Proof. The fact that the bracket $(f, g) \mapsto \{f, g\}_\Theta$ on $C^\infty(\mathcal{G}^*, \mathbb{R})$ is a Poisson bracket was already indicated in 4.4.3. It can be verified by easy calculations. The fact that J is a Poisson map can be proven by first looking at linear functions on \mathcal{G}^* , *i.e.* elements in \mathcal{G} . The reader will find a detailed proof in [38]. \square

5.5.4 Remark. When the momentum map J is replaced by another momentum map $J_1 = J + \mu$, where $\mu \in \mathcal{G}^*$ is a constant, the symplectic Lie group cocycle θ and the symplectic Lie algebra cocycle Θ are replaced by θ_1 and Θ_1 , respectively, given by

$$\begin{aligned}\theta_1(g) &= \theta(g) + \mu - \text{Ad}_{g^{-1}}^*(\mu), \quad g \in G, \\ \Theta_1(X, Y) &= \Theta(X, Y) + \langle \mu, [X, Y] \rangle, \quad X \text{ and } Y \in \mathcal{G}.\end{aligned}$$

These formulae show that $\theta_1 - \theta$ and $\Theta_1 - \Theta$ are *symplectic coboundaries* of the Lie group G and the Lie algebra \mathcal{G} . In other words, the *cohomology classes* of the cocycles θ and Θ only depend on the Hamiltonian action Φ of G on the symplectic manifold (M, ω) .

5.6 The use of symmetries in Hamiltonian Mechanics

5.6.1 Symmetries of the phase space

Hamiltonian Symmetries are often used for the search of solutions of the equations of motion of mechanical systems. The symmetries considered are those of the *phase space* of the mechanical system. This space is very often a *symplectic manifold*, either the cotangent bundle to the configuration space with its canonical symplectic structure, or a more general symplectic manifold. Sometimes, after some simplifications, the phase space is a *Poisson manifold*.

The *Marsden-Weinstein reduction procedure* [39, 43] or one of its generalizations [45] is the method most often used to facilitate the determination of solutions of the equations of motion. In a first step, a possible value of the momentum map is chosen and the subset of the phase space on which the momentum map takes this value is determined. In a second step, that subset (when it is a smooth manifold) is quotiented by its isotropic foliation. The quotient manifold is a symplectic manifold of a dimension smaller than that of the original phase space, and one has an easier to solve Hamiltonian system on that reduced phase space.

When Hamiltonian symmetries are used for the reduction of the dimension of the phase space of a mechanical system, the symplectic cocycle of the Lie group of symmetries action, or of the Lie algebra of symmetries action, is almost always the *zero cocycle*.

For example, if the group of symmetries is the canonical lift to the cotangent bundle of a group of symmetries of the configuration space, not only the *canonical symplectic form*, but the *Liouville 1-form* of the cotangent bundle itself remains invariant under the action of the symmetry group, and this fact implies that the symplectic cohomology class of the action is zero.

5.6.2 Symmetries of the space of motions

A completely different way of using symmetries was initiated by Jean-Marie Souriau, who proposed to consider the symmetries of the *manifold of motions* of the mechanical system. He observed that the Lagrangian and Hamiltonian formalisms, in their usual formulations, *involve the choice of a particular reference frame*, in which the motion is described. This choice *destroys a part of the natural symmetries of the system*.

For example, in classical (non-relativistic) Mechanics, the natural symmetry group of an isolated mechanical system must contain the symmetry group of the *Galilean space-time*, called the *Galilean group*. This group is of *dimension 10*. It contains not only the *group of Euclidean displacements of space* which is of *dimension 6* and the *group of time translations* which is of *dimension 1*, but the *group of linear changes of Galilean reference frames* which is of *dimension 3*.

If we use the *Lagrangian formalism* or the *Hamiltonian formalism*, the Lagrangian or the Hamiltonian of the system *depends on the reference frame: it is not invariant with respect to linear changes of Galilean reference frames*.

It may seem strange to consider the set of all possible motions of a system, which is unknown as long as we have not determined all these possible motions. One may ask if it is really useful when we want to determine not all possible motions, but only one motion with prescribed initial data, since that motion is just one point of the (unknown) manifold of motion!

Souriau's answers to this objection are the following.

1. We know that the manifold of motions has a *symplectic structure*, and very often many things are known about its *symmetry properties*.
2. In classical (non-relativistic) mechanics, there exists a natural mathematical object which *does not depend on the choice of a particular reference frame* (even if the descriptions given to that object by different observers depend on the reference frames used by these observers): it is the *evolution space* of the system.

The knowledge of the equations which govern the system's evolution allows the full mathematical description of the *evolution space*, even when these equations are not yet solved.

Moreover, the symmetry properties of the *evolution space* are the same as those of the manifold of motions.

For example, the *evolution space* of a classical mechanical system with configuration manifold N is

1. in the Lagrangian formalism, the space $\mathbb{R} \times TN$ endowed with the presymplectic form $d\widehat{\omega}_L$, whose kernel is of dimension 1 when the Lagrangian L is hyper-regular,
2. in the Hamiltonian formalism, the space $\mathbb{R} \times T^*N$ with the presymplectic form $d\widehat{\omega}_H$, whose kernel too is of dimension 1.

The Poincaré-Cartan 1-form $\widehat{\omega}_L$ in the Lagrangian formalism, or $\widehat{\omega}_H$ in the Hamiltonian formalism, depends on the choice of a particular reference frame, made for using the Lagrangian or the Hamiltonian formalism. But their exterior differentials, the presymplectic forms $d\widehat{\omega}_L$ or $d\widehat{\omega}_H$, *do not depend on that choice*, modulo a simple change of variables in the evolution space.

Souriau defined this presymplectic form in a framework more general than those of Lagrangian or Hamiltonian formalisms, and called it the *Lagrange form*. In this more general setting, it may not be an exact 2-form. Souriau proposed as a new *Principle*, the assumption that it always projects on the space of motions of the system as a *symplectic form*, even in Relativistic Mechanics in which the definition of an evolution space is not clear. He called this new principle the *Maxwell Principle*.

V. Bargmann proved that the symplectic cohomology of the Galilean group is of dimension 1, and Souriau proved that the cohomology class of its action on the manifold

of motions of an isolated classical (non-relativistic) mechanical system can be identified with the *total mass* of the system ([55], chapter III, page 153).

Readers interested in the Galilean group and momentum maps of its actions are referred to the recent book by G. de Saxcé and C. Vallée [52].

6 Statistical Mechanics and Thermodynamics

6.1 Basic concepts in Statistical Mechanics

During the XVIII–th and XIX–th centuries, the idea that material bodies (fluids as well as solids) are assemblies of a very large number of small, moving particles, began to be considered by some scientists, notably Daniel Bernoulli (1700–1782), Rudolf Clausius (1822–1888), James Clerk Maxwell (1831–1879) and Ludwig Eduard Boltzmann (1844–1906), as a reasonable possibility. Attempts were made to explain the nature of some measurable macroscopic quantities (for example the temperature of a material body, the pressure exerted by a gas on the walls of the vessel in which it is contained), and the laws which govern the variations of these macroscopic quantities, by application of the laws of Classical Mechanics to the motions of these very small particles. Described in the framework of the Hamiltonian formalism, the material body is considered as a Hamiltonian system whose phase space is a very high dimensional symplectic manifold (M, ω) , since an element of that space gives a perfect information about the positions and the velocities of all the particles of the system. The experimental determination of the exact state of the system being impossible, one only can use the probability of presence, at each instant, of the state of the system in various parts of the phase space. Scientists introduced the concept of a *statistical state*, defined below.

6.1.1 Definition. Let (M, ω) be a symplectic manifold. A *statistical state* is a probability measure μ on the manifold M .

6.1.2 The Liouville measure on a symplectic manifold

On each symplectic manifold (M, ω) , with $\dim M = 2n$, there exists a positive measure λ_ω , called the *Liouville measure*. Let us briefly recall its definition. Let (U, φ) be a Darboux chart of (M, ω) (4.4.1). The open subset U of M is, by means of the diffeomorphism φ , identified with an open subset $\varphi(U)$ of \mathbb{R}^{2n} on which the coordinates (Darboux coordinates) will be denoted by $(p_1, \dots, p_n, x^1, \dots, x^n)$. With this identification, the Liouville measure (restricted to U) is simply the Lebesgue measure on the open subset $\varphi(U)$ of \mathbb{R}^{2n} . In other words, for each Borel subset A of M contained in U , we have

$$\lambda_\omega(A) = \int_{\varphi(A)} dp_1 \dots dp_n dx^1 \dots dx^n.$$

One can easily check that this definition does not depend on the choice of the Darboux coordinates $(p_1, \dots, p_n, x^1, \dots, x^n)$ on $\varphi(A)$. By using an atlas of Darboux charts on (M, ω) , one can easily define $\lambda_\omega(A)$ for any Borel subset A of M .

6.1.3 Definition. A statistical state μ on the symplectic manifold (M, ω) is said to be *continuous* (respectively, is said to be *smooth*) if it has a continuous (respectively, a smooth) density with respect to the Liouville measure λ_ω , *i.e.* if there exists a continuous function (respectively, a smooth function) $\rho : M \rightarrow \mathbb{R}$ such that, for each Borel subset A of M

$$\mu(A) = \int_A \rho d\lambda_\omega.$$

6.1.4 Remark. The density ρ of a continuous statistical state on (M, ω) takes its values in \mathbb{R}^+ and of course satisfies

$$\int_M \rho d\lambda_\omega = 1.$$

For simplicity we only consider in what follows continuous, very often even smooth statistical states.

6.1.5 Variation in time of a statistical state

Let H be a smooth time independent Hamiltonian on a symplectic manifold (M, ω) , X_H the associated Hamiltonian vector field and Φ^{X_H} its reduced flow. We consider the mechanical system whose time evolution is described by the flow of X_H .

If the state of the system at time t_0 , assumed to be perfectly known, is a point $z_0 \in M$, its state at time t_1 is the point $z_1 = \Phi_{t_1-t_0}^{X_H}(z_0)$.

Let us now assume that the state of the system at time t_0 is not perfectly known, but that a continuous probability measure on the phase space M , whose density with respect to the Liouville measure λ_ω is ρ_0 , describes the probability distribution of presence of the state of the system at time t_0 . In other words, ρ_0 is the density of the statistical state of the system at time t_0 . For any other time t_1 , the map $\Phi_{t_1-t_0}^{X_H}$ is a symplectomorphism, therefore leaves invariant the Liouville measure λ_ω . The probability density ρ_1 of the statistical state of the system at time t_1 therefore satisfies, for any $x_0 \in M$ for which $x_1 = \Phi_{t_1-t_0}^{X_H}(x_0)$ is defined,

$$\rho_1(x_1) = \rho_1(\Phi_{t_1-t_0}^{X_H}(x_0)) = \rho_0(x_0).$$

Since $(\Phi_{t_1-t_0}^{X_H})^{-1} = \Phi_{t_0-t_1}^{X_H}$, we can write

$$\rho_1 = \rho_0 \circ \Phi_{t_0-t_1}^{X_H}.$$

6.1.6 Definition. Let ρ be the density of a continuous statistical state μ on the symplectic manifold (M, ω) . The number

$$s(\rho) = \int_M \rho \log \left(\frac{1}{\rho} \right) d\lambda_\omega$$

is called the *entropy* of the statistical state μ or, with a slight abuse of language, the *entropy* of the density ρ .

6.1.7 Remarks.

1. By convention we state that $0 \log \left(\frac{1}{0} \right) = 0$. With that convention the function $x \mapsto x \log \left(\frac{1}{x} \right)$ is continuous on \mathbb{R}^+ . If the integral on the right hand side of the equality which defines $s(\rho)$ does not converge, we state that $s(\rho) = -\infty$. With these conventions, $s(\rho)$ exists for any continuous probability density ρ .
2. The above definition (6.1.6) of the entropy of a statistical state, founded on ideas developed by Boltzmann in his Kinetic Theory of Gases [9], specially in the derivation of his famous (and controverted) *Theorem Éta*, is too related with the ideas of Claude Shannon [53] on Information theory. The use of Information theory in Thermodynamics was more recently proposed by Jaynes [21, 22] and Mackey [34]. For a very nice discussion of the use of probability concepts in Physics and application of Information theory in Quantum Mechanics, the reader is referred to the paper by R. Balian [3].

The entropy $s(\rho)$ of a probability density ρ has very remarkable variational properties discussed in the following definitions and proposition.

6.1.8 Definitions. Let ρ be the density of a smooth statistical state on a symplectic manifold (M, ω) .

1. For each function f defined on M , taking its values in \mathbb{R} or in some finite-dimensional vector space, such that the integral on the right hand side of the equality

$$\mathcal{E}_\rho(f) = \int_M f \rho d\lambda_\omega$$

converges, the value $\mathcal{E}_\rho(f)$ of that integral is called the *mean value of f with respect to ρ* .

2. Let f be a smooth function on M , taking its values in \mathbb{R} or in some finite-dimensional vector space, satisfying the properties stated above. A *smooth infinitesimal variation of ρ with fixed mean value of f* is a smooth map, defined on the product $] - \varepsilon, \varepsilon[\times M$, with values in \mathbb{R}^+ , where $\varepsilon > 0$,

$$(\tau, z) \mapsto \rho(\tau, z), \quad \tau \in] - \varepsilon, \varepsilon[, \quad z \in M,$$

such that

- for $\tau = 0$ and any $z \in M$, $\rho(0, z) = \rho(z)$,
- for each $\tau \in] - \varepsilon, \varepsilon[$, $z \mapsto \rho_\tau(z) = \rho(\tau, z)$ is a smooth probability density on M such that

$$\mathcal{E}_{\rho_\tau}(f) = \int_M \rho_\tau f d\lambda_\omega = \mathcal{E}_\rho(f).$$

3. The entropy function s is said to be *stationary* at the probability density ρ with respect to smooth infinitesimal variations of ρ with fixed mean value of f , if for any smooth infinitesimal variation $(\tau, z) \mapsto \rho(\tau, z)$ of ρ with fixed mean value of f

$$\left. \frac{ds(\rho_\tau)}{d\tau} \right|_{\tau=0} = 0.$$

6.1.9 Proposition. Let $H : M \rightarrow \mathbb{R}$ be a smooth Hamiltonian on a symplectic manifold (M, ω) and ρ be the density of a smooth statistical state on M such that the integral defining the mean value $\mathcal{E}_\rho(H)$ of H with respect to ρ converges. The entropy function s is stationary at ρ with respect to smooth infinitesimal variations of ρ with fixed mean value of H , if and only if there exists a real $b \in \mathbb{R}$ such that, for all $z \in M$,

$$\rho(z) = \frac{1}{P(b)} \exp(-bH(z)), \quad \text{with } P(b) = \int_M \exp(-bH) d\lambda_\omega.$$

Proof. Let $\tau \mapsto \rho_\tau$ be a smooth infinitesimal variation of ρ with fixed mean value of H .

Since $\int_M \rho_\tau d\lambda_\omega$ and $\int_M \rho_\tau H d\lambda_\omega$ do not depend on τ , it satisfies, for all $\tau \in] - \varepsilon, \varepsilon[$,

$$\int_M \frac{\partial \rho(\tau, z)}{\partial \tau} d\lambda_\omega(z) = 0, \quad \int_M \frac{\partial \rho(\tau, z)}{\partial \tau} H(z) d\lambda_\omega(z) = 0.$$

Moreover an easy calculation leads to

$$\left. \frac{ds(\rho_\tau)}{d\tau} \right|_{\tau=0} = - \int_M \left. \frac{\partial \rho(\tau, z)}{\partial \tau} \right|_{\tau=0} (1 + \log(\rho(z))) d\lambda_\omega(z).$$

A well known result in calculus of variations shows that the entropy function s is stationary at ρ with respect to smooth infinitesimal variations of ρ with fixed mean value of H , if and only if there exist two real constants a and b , called *Lagrange multipliers*, such that, for all $z \in M$,

$$1 + \log(\rho) + a + bH = 0,$$

which leads to

$$\rho = \exp(-1 - a - bH).$$

By writing that $\int_M \rho d\lambda_\omega = 1$, we see that a is determined by b :

$$\exp(1 + a) = P(b) = \int_M \exp(-bH) d\lambda_\omega. \quad \square$$

6.1.10 Definitions. Let $H : M \rightarrow \mathbb{R}$ be a smooth Hamiltonian on a symplectic manifold (M, ω) . For each $b \in \mathbb{R}$ such that the integral on the right side of the equality

$$P(b) = \int_M \exp(-bH) d\lambda_\omega$$

converges, the smooth probability measure on M with density (with respect to the Liouville measure)

$$\rho(b) = \frac{1}{P(b)} \exp(-bH)$$

is called the *Gibbs statistical state* associated to b . The function $P : b \mapsto P(b)$ is called the *partition function*.

The following proposition shows that the entropy function, not only is stationary at any Gibbs statistical state, but in a certain sense attains at that state a strict maximum.

6.1.11 Proposition. Let $H : M \rightarrow \mathbb{R}$ be a smooth Hamiltonian on a symplectic manifold (M, ω) and $b \in \mathbb{R}$ be such that the integral defining the value $P(b)$ of the partition function P at b converges. Let

$$\rho_b = \frac{1}{P(b)} \exp(-bH)$$

be the probability density of the Gibbs statistical state associated to b . We assume that the Hamiltonian H is bounded by below, i.e. that there exists a constant m such that $m \leq H(z)$ for any $z \in M$. Then the integral defining

$$\mathcal{E}_{\rho_b}(H) = \int_M \rho_b H d\lambda_\omega$$

converges. For any other smooth probability density ρ_1 such that

$$\mathcal{E}_{\rho_1}(H) = \mathcal{E}_{\rho_b}(H),$$

we have

$$s(\rho_1) \leq s(\rho_b),$$

and the equality $s(\rho_1) = s(\rho_b)$ holds if and only if $\rho_1 = \rho_b$.

Proof. Since $m \leq H$, the function $\rho_b \exp(-bH)$ satisfies $0 \leq \rho_b \exp(-bH) \leq \exp(-mb)\rho_b$, therefore is integrable on M . Let ρ_1 be any smooth probability density on M satisfying $\mathcal{E}_{\rho_1}(H) = \mathcal{E}_{\rho_b}(H)$. The function defined on \mathbb{R}^+

$$x \mapsto h(x) = \begin{cases} x \log \left(\frac{1}{x} \right) & \text{if } x > 0 \\ 0 & \text{if } x = 0 \end{cases}$$

being convex, its graph is below the tangent at any of its points $(x_0, h(x_0))$. We therefore have, for all $x > 0$ and $x_0 > 0$,

$$h(x) \leq h(x_0) - (1 + \log x_0)(x - x_0) = x_0 - x(1 + \log x_0).$$

With $x = \rho_1(z)$ and $x_0 = \rho_b(z)$, z being any element in M , that inequality becomes

$$h(\rho_1(z)) = \rho_1(z) \log \left(\frac{1}{\rho_1(z)} \right) \leq \rho_b(z) - (1 + \log \rho_b(z))\rho_1(z).$$

By integration over M , using the fact that ρ_b is the probability density of the Gibbs state associated to b , we obtain

$$s(\rho_1) \leq 1 - 1 - \int_M \rho_1 \log \rho_b d\lambda_\omega = s(\rho_b).$$

We have proven the inequality $s(\rho_1) \leq s(\rho_b)$. If $\rho_1 = \rho_b$, we have of course the equality $s(\rho_1) = s(\rho_b)$. Conversely if $s(\rho_1) = s(\rho_b)$, the functions defined on M

$$z \mapsto \varphi_1(z) = \rho_1(z) \log \left(\frac{1}{\rho_1(z)} \right) \quad \text{and} \quad z \mapsto \varphi(z) = \rho_b(z) - (1 + \log \rho_b(z))\rho_1(z)$$

are continuous on M except, maybe, for φ , at points z at which $\rho_b(z) = 0$ and $\rho_1(z) \neq 0$, but the set of such points is of measure 0 since φ is integrable. They satisfy the inequality $\varphi_1 \leq \varphi$. Both are integrable on M and have the same integral. The function $\varphi - \varphi_1$ is everywhere ≥ 0 , is integrable on M and its integral is 0. That function is therefore everywhere equal to 0 on M . We can write, for any $z \in M$,

$$\rho_1(z) \log \left(\frac{1}{\rho_1(z)} \right) = \rho_b(z) - (1 + \log \rho_b(z))\rho_1(z). \quad (*)$$

For each $z \in M$ such that $\rho_1(z) \neq 0$, we can divide that equality by $\rho_1(z)$. We obtain

$$\frac{\rho_b(z)}{\rho_1(z)} - \log \left(\frac{\rho_b(z)}{\rho_1(z)} \right) = 1.$$

Since the function $x \mapsto x - \log x$ reaches its minimum, equal to 1, for a unique value of $x > 0$, that value being 1, we see that for each $z \in M$ at which $\rho_1(z) > 0$, we have $\rho_1(z) = \rho_b(z)$. At points $z \in M$ at which $\rho_1(z) = 0$, the above equality (*) shows that $\rho_b(z) = 0$. Therefore $\rho_1 = \rho_b$. \square

The following proposition shows that a Gibbs statistical state remains invariant under the flow of the Hamiltonian vector field X_H . In that sense, one can say that a Gibbs statistical state is a statistical equilibrium state. Of course, there exist statistical states which remain invariant under the flow of X_H other than Gibbs states.

6.1.12 Proposition. *Let H be a smooth Hamiltonian bounded by below on a symplectic manifold (M, ω) , $b \in \mathbb{R}$ be such that the integral defining the value $P(b)$ of the partition function P at b converges. The Gibbs state associated to b remains invariant under the flow of the Hamiltonian vector field X_H .*

Proof. The density ρ_b of the Gibbs state associated to b , with respect to the Liouville measure λ_ω , is

$$\rho_b = \frac{1}{P(b)} \exp(-bH).$$

Since H is constant along each integral curve of X_H , ρ_b too is constant along each integral curve of X_H . Moreover, the Liouville measure λ_ω remains invariant under the flow of X_H . Therefore the Gibbs probability measure associated to b too remains invariant under that flow. \square

6.2 Thermodynamic equilibria and thermodynamic functions

6.2.1 Assumptions made in this section.

Any Hamiltonian H defined on a symplectic manifold (M, ω) considered in this section will be assumed to be smooth, bounded by below and such that for any real $b > 0$, each one of the three functions, defined on M , $z \mapsto \exp(-bH(z))$, $z \mapsto |H(z)| \exp(-bH(z))$ and $z \mapsto (H(z))^2 \exp(-bH(z))$ is everywhere smaller than some function defined on M integrable with respect to the Liouville measure λ_ω . The integrals which define

$$P(b) = \int_M \exp(-bH) d\lambda_\omega \quad \text{and} \quad \mathcal{E}_{\rho_b}(H) = \int_M H \exp(-bH) d\lambda_\omega$$

therefore converge.

6.2.2 Proposition. *Let H be a Hamiltonian defined on a symplectic manifold (M, ω) satisfying the assumptions indicated in 6.2.1. For any real $b > 0$ let*

$$P(b) = \int_M \exp(-bH) d\lambda_\omega \quad \text{and} \quad \rho_b = \frac{1}{P(b)} \exp(-bH)$$

be the value at b of the partition function P and the probability density of the Gibbs statistical state associated to b , and

$$E(b) = \mathcal{E}_{\rho_b}(H) = \frac{1}{P(b)} \int_M H \exp(-bH) d\lambda_\omega$$

be the mean value of H with respect to the probability density ρ_b . The first and second derivatives with respect to b of the partition function P exist, are continuous functions of b given by

$$\frac{dP(b)}{db} = -P(b)E(b), \quad \frac{d^2P(b)}{db^2} = \int_M H^2 \exp(-bH) d\lambda_\omega = P(b)\mathcal{E}_{\rho_b}(H^2).$$

The derivative with respect to b of the function E exists and is a continuous function of b given by

$$\frac{dE(b)}{db} = -\frac{1}{P(b)} \int_M (H - \mathcal{E}_{\rho_b}(H))^2 d\lambda_\omega = -\mathcal{E}_{\rho_b} \left((H - \mathcal{E}_{\rho_b}(H))^2 \right).$$

We have always $\frac{dE(b)}{db} \leq 0$, and when H is not a constant function on M , $\frac{dE(b)}{db} < 0$.

Let $S(b)$ be the entropy $s(\rho_b)$ of the Gibbs statistical state associated to b . The function S can be expressed in terms of P and E as

$$S(b) = \log(P(b)) + bE(b).$$

Its derivative with respect to b exists and is a continuous function of b given by

$$\frac{dS(b)}{db} = b \frac{dE(b)}{db}.$$

Proof. Using the assumptions 6.2.1, we see that the functions $b \mapsto P(b)$ and $b \mapsto \mathcal{E}_{\rho_b}(H) = E(b)$, defined by integrals on M , have a derivative with respect to b which is continuous and which can be calculated by derivation under the sign \int_M . The indicated results easily follow, if we observe that for any function f on M such that $\mathcal{E}_{\rho_b}(f)$ and $\mathcal{E}_{\rho_b}(f^2)$ exist, we have the formula, well known in Probability theory,

$$\mathcal{E}_{\rho_b}(f^2) - (\mathcal{E}_{\rho_b}(f))^2 = \mathcal{E}_{\rho_b}\left((f - \mathcal{E}_{\rho_b}(f))^2\right).$$

We have always $\frac{dE(b)}{db} \leq 0$, the inequality being strict when H is not a constant function on M , since that quantity is the opposite of the mean value of a continuous non-negative function, not everywhere 0 when H is not a constant function on M . \square

6.2.3 Physical meaning of the introduced functions

Let us consider a physical system, for example a gas contained in a vessel bounded by rigid, thermally insulated walls, at rest in a Galilean reference frame. We assume that its evolution can be mathematically described by means of a Hamiltonian system on a symplectic manifold (M, ω) whose Hamiltonian H satisfies the assumptions 6.2.1. For physicists, a Gibbs statistical state, *i.e.* a probability measure of density $\rho_b = \frac{1}{P(b)} \exp(-bH)$ on M , is a *thermodynamic equilibrium* of the physical system. The set of possible thermodynamic equilibria of the system is therefore indexed by a real parameter $b > 0$. The following argument will show what physical meaning can have that parameter.

Let us consider two similar physical systems, mathematically described by two Hamiltonian systems, of Hamiltonians H_1 on the symplectic manifold (M_1, ω_1) and H_2 on the symplectic manifold (M_2, ω_2) . We first assume that they are independent and both in thermodynamic equilibrium, with different values b_1 and b_2 of the parameter b . We denote by $E_1(b_1)$ and $E_2(b_2)$ the mean values of H_1 on the manifold M_1 with respect to the Gibbs state of density ρ_{1,b_1} and of H_2 on the manifold M_2 with respect to the Gibbs state of density ρ_{2,b_2} . We assume now that the two systems are coupled in a way allowing an exchange of energy. For example, the two vessels containing the two gases can be separated by a wall allowing a heat transfer between them. Coupled together, they make a new physical system, mathematically described by a Hamiltonian system on the symplectic manifold $(M_1 \times M_2, p_1^* \omega_1 + p_2^* \omega_2)$, where $p_1 : M_1 \times M_2 \rightarrow M_1$ and $p_2 : M_1 \times M_2 \rightarrow M_2$ are the canonical projections. The Hamiltonian of this new system can be made as close to $H_1 \circ p_1 + H_2 \circ p_2$ as one wishes, by making very small the coupling between the two systems. The mean value of the Hamiltonian of the new system is therefore very close to

$E_1(b_1) + E_2(b_2)$. When the total system will reach a state of thermodynamic equilibrium, the probability densities of the Gibbs states of its two parts, $\rho_{1,b'}$ on M_1 and $\rho_{2,b'}$ on M_2 will be indexed by the same real number $b' > 0$, which must be such that

$$E_1(b') + E_2(b') = E_1(b_1) + E_2(b_2).$$

By 6.2.2, we have, for all $b > 0$,

$$\frac{dE_1(b)}{db} \leq 0, \quad \frac{dE_2(b)}{db} \leq 0.$$

Therefore b' must lie between b_1 and b_2 . If, for example, $b_1 < b_2$, we see that $E_1(b') \leq E_1(b_1)$ and $E_2(b') \geq E_2(b_2)$. In order to reach a state of thermodynamic equilibrium, energy must be transferred from the part of the system where b has the smallest value, towards the part of the system where b has the highest value, until, at thermodynamic equilibrium, b has the same value everywhere. Everyday experience shows that thermal energy flows from parts of a system where the temperature is higher, towards parts where it is lower. For this reason physicists consider the real variable b as a way to appreciate the temperature of a physical system in a state of thermodynamic equilibrium. More precisely, they state that

$$b = \frac{1}{kT}$$

where T is the absolute temperature and k a constant depending on the choice of units of energy and temperature, called *Boltzmann's constant* in honour of the great Austrian scientist Ludwig Eduard Boltzmann (1844–1906).

For a physical system mathematically described by a Hamiltonian system on a symplectic manifold (M, ω) , with H as Hamiltonian, in a state of thermodynamic equilibrium, $E(b)$ and $S(b)$ are the *internal energy* and the *entropy* of the system.

6.2.4 Towards thermodynamic equilibrium

Everyday experience shows that a physical system, when submitted to external conditions which remain unchanged for a sufficiently long time, very often reaches a state of thermodynamic equilibrium. At first look, when perfectly defined states are considered, it seems that Lagrangian or Hamiltonian systems with time-independent Lagrangians or Hamiltonians cannot exhibit a similar behaviour. Let us indeed consider a mechanical system whose configuration space is a smooth manifold N , described in the Lagrangian formalism by a smooth time-independent hyper-regular Lagrangian $L : TN \rightarrow \mathbb{R}$ or, in the Hamiltonian formalism, by the associated Hamiltonian $H_L : T^*N \rightarrow \mathbb{R}$. Let $t \mapsto \overrightarrow{x(t)}$ be a motion of that system, $\overrightarrow{x_0} = \overrightarrow{x(t_0)}$ and $\overrightarrow{x_1} = \overrightarrow{x(t_1)}$ be the configurations of the system for that motion at times t_0 and t_1 . There exists another motion $t \mapsto \overrightarrow{x'(t)}$ of the system for which $\overrightarrow{x'(t_0)} = \overrightarrow{x_1}$ and $\overrightarrow{x'(t_1)} = \overrightarrow{x_0}$: since the equations of motion are invariant by time reversal, the motion $t \mapsto \overrightarrow{x'(t)}$ is obtained simply by taking as initial condition at time t_0 $\overrightarrow{x'(t_0)} = \overrightarrow{x_1}$ and $\left. \frac{d\overrightarrow{x'(t)}}{dt} \right|_{t=t_0} = -\left. \frac{d\overrightarrow{x(t)}}{dt} \right|_{t=t_1}$. Another more serious argument against a kind of thermodynamic behaviour of Lagrangian or Hamiltonian systems rests on the famous recurrence theorem due to H. Poincaré [46]. This theorem asserts indeed that when the useful part of the phase space of the system is of a finite total measure, almost all points in an arbitrarily small open subset of the phase space are recurrent, *i.e.*, the motion

starting of such a point at time t_0 repeatedly crosses that open subset again and again, infinitely many times when $t \rightarrow +\infty$.

If instead of perfectly defined states, *i.e.*, points in phase space, we now consider statistical states, it is not so obvious that a Lagrangian or Hamiltonian system, with a time-independent Lagrangian or Hamiltonian, starting at time t_0 from a given statistical state, cannot evolve in such a way that its statistical state converges, when $t \rightarrow +\infty$, towards an equilibrium statistical state, and more precisely towards a Gibbs statistical state. Of course we should specify in what sense, of for which topology, such a convergence may occur, and what physical meaning should be given to a statistical state of a physical system. A positive partial answer was given by Ludwig Boltzmann when, developing his kinetic theory of gases, he proved his famous (but controverted) *Êta theorem* stating that the entropy of the statistical state of a gas of small particles is a monotonously increasing function of time. This question, linked with ergodic theory and with the problem of time irreversibility in Physics, is still the subject of important researches, both by physicists and by mathematicians. Many physicists however consider that question of academic interest only, because the behaviour of particules is only approximately described by the laws of Classical Mechanics. They think that the question must be dealt with in the framework of Quantum Mechanics, which only provides probability estimates and offers a more accurate description of their behaviour. The reader is referred to the paper [3] by R. Balian for a more thorough discussion of that question.

6.3 Examples of thermodynamic equilibria

6.3.1 Classical monoatomic ideal gas

In Classical Mechanics, a dilute gas contained in a vessel at rest in a Galilean reference frame is mathematically described by a Hamiltonian system made by a large number of very small massive particles, which interact by very brief collisions between themselves or with the walls of the vessel, whose motions between two collisions are free. Let us first assume that these particles are material points and that no external field is acting on them, other than that describing the interactions by collisions with the walls of the vessel.

The Hamiltonian of one particle in a part of the phase space in which its motion is free is simply

$$\frac{1}{2m} \|\vec{p}\|^2 = \frac{1}{2m} (p_1^2 + p_2^2 + p_3^2), \quad \text{with} \quad \vec{p} = m \vec{v},$$

where m is the mass of the particle, \vec{v} its velocity vector and \vec{p} its linear momentum vector (in the considered Galilean reference frame), p_1 , p_2 and p_3 the components of \vec{p} in a fixed orthonormal basis of the physical space.

Let N be the total number of particles, which may not have all the same mass. We use a integer $i \in \{1, 2, \dots, N\}$ to label the particles and denote by m_i , \vec{x}_i , \vec{v}_i , \vec{p}_i the mass and the vectors position, velocity and linear momentum of the i -th particle.

The Hamiltonian of the gas is therefore

$$H = \sum_{i=1}^N \frac{1}{2m_i} \|\vec{p}_i\|^2 + \text{terms involving the collisions between particles and with the walls.}$$

Interactions of the particles with the walls of the vessel are essential for allowing the motions of particles to remain confined. Interactions between particles are essential to allow the exchanges between them of energy and momentum, which play an important

part in the evolution with time of the statistical state of the system. However it appears that while these terms are very important to determine the system's evolution with time, they can be neglected, when the gas is dilute enough, if we only want to determine the final statistical state of the system, once a thermodynamic equilibrium is established. The Hamiltonian used will therefore be

$$H = \sum_{i=1}^N \frac{1}{2m_i} \|\vec{p}_i\|^2.$$

The partition function is

$$P(b) = \int_M \exp(-bH) d\lambda_\omega = \int_D \exp\left(-b \sum_{i=1}^N \frac{1}{2m_i} \|\vec{p}_i\|^2\right) \prod_{i=1}^N (d\vec{x}_i d\vec{p}_i),$$

where D is the domain of the $6N$ -dimensional space spanned by the position vectors \vec{x}_i and linear momentum vectors \vec{p}_i of the particles in which all the \vec{x}_i lie within the vessel containing the gas. An easy calculation leads to

$$P(b) = V^N \left(\frac{2\pi}{b}\right)^{3N/2} \prod_{i=1}^N (m_i^{3/2}) = \prod_{i=1}^N \left[V \left(\frac{2\pi m_i}{b}\right)^{3/2} \right],$$

where V is the volume of the vessel which contains the gas. The probability density of the Gibbs state associated to b , with respect to the Liouville measure, therefore is

$$\rho_b = \prod_{i=1}^N \left[\frac{1}{V} \left(\frac{b}{2\pi m_i}\right)^{3/2} \exp\left(\frac{-b\|\vec{p}_i\|^2}{2m_i}\right) \right].$$

We observe that ρ_b is the product of the probability densities $\rho_{i,b}$ for the i -th particle

$$\rho_{i,b} = \frac{1}{V} \left(\frac{b}{2\pi m_i}\right)^{3/2} \exp\left(\frac{-b\|\vec{p}_i\|^2}{2m_i}\right).$$

The $2N$ stochastic vectors \vec{x}_i and \vec{p}_i , $i = 1, \dots, N$ are therefore independent. The position \vec{x}_i of the i -th particle is uniformly distributed in the volume of the vessel, while the probability measure of its linear momentum \vec{p}_i is the classical *Maxwell-Boltzmann probability distribution of linear momentum* for an ideal gas of particles of mass m_i , first obtained by Maxwell in 1860. Moreover we see that the three components p_{i1} , p_{i2} and p_{i3} of the linear momentum \vec{p}_i in an orthonormal basis of the physical space are independent stochastic variables.

By using the formulae given in 6.2.2 the internal energy $E(b)$ and the entropy $S(b)$ of the gas can be easily deduced from the partition function $P(b)$. Their expressions are

$$E(b) = \frac{3N}{2b}, \quad S(b) = \frac{3}{2} \sum_{i=1}^N \log m_i + \left(\frac{3}{2}(1 + \log(2\pi)) + \log V\right) N - \frac{3N}{2} \log b.$$

We see that each of the N particles present in the gas has the same contribution $\frac{3}{2b}$ to the internal energy $E(b)$, which does not depend on the mass of the particle. Even more: each degree of freedom of each particle, *i.e.* each of the the three components of the the linear momentum of the particle on the three axes of an orthonormal basis, has the

same contribution $\frac{1}{2b}$ to the internal energy $E(b)$. This result is known in Physics under the name *Theorem of equipartition of the energy at a thermodynamic equilibrium*. It can be easily generalized for polyatomic gases, in which a particle may carry, in addition to the kinetic energy due to the velocity of its centre of mass, a kinetic energy due to the particle's rotation around its centre of mass. The reader can consult the books by Souriau [55] and Mackey [34] where the kinetic theory of polyatomic gases is discussed.

The pressure in the gas, denoted by $\Pi(b)$ because the notation $P(b)$ is already used for the partition function, is due to the change of linear momentum of the particles which occurs at a collision of the particle with the walls of the vessel containing the gas (or with a probe used to measure that pressure). A classical argument in the kinetic theory of gases (see for example [13] or [14]) leads to

$$\Pi(b) = \frac{2}{3} \frac{E(b)}{V} = \frac{N}{bV}.$$

This formula is the well known *equation of state* of an ideal monoatomic gas relating the number of particles by unit of volume, the pressure and the temperature.

With $b = \frac{1}{kT}$, the above expressions are exactly those used in classical Thermodynamics for an ideal monoatomic gas.

6.3.2 Classical ideal monoatomic gas in a gravity field

Let us now assume that the gas, contained in a cylindrical vessel of section Σ and length h , with a vertical axis, is submitted to the vertical gravity field of intensity g directed downwards. We choose Cartesian coordinates x, y, z , the z axis being vertical directed upwards, the bottom of the vessel being in the horizontal surface $z = 0$. The Hamiltonian of a free particle of mass m , position and linear momentum vectors \vec{x} (components x, y, z) and \vec{p} (components p_x, p_y and p_z) is

$$\frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + mgz.$$

As in the previous section we neglect the parts of the Hamiltonian of the gas corresponding to collisions between the particles, or between a particle and the walls of the vessel. The Hamiltonian of the gas is therefore

$$H = \sum_{i=1}^N \left(\frac{1}{2m_i}(p_{ix}^2 + p_{iy}^2 + p_{iz}^2) + m_i g z_i \right).$$

Calculations similar to those of the previous section lead to

$$P(b) = \prod_{i=1}^N \left[\Sigma \left(\frac{2\pi m_i}{b} \right)^{3/2} \frac{1 - \exp(-m_i g b h)}{m_i g b} \right],$$

$$\rho_b = \frac{1}{P(b)} \exp \left[-b \sum_{i=1}^N \left(\frac{\|\vec{p}_i\|^2}{2m_i} + m_i g z_i \right) \right].$$

The expression of ρ_b shows that the $2N$ stochastic vectors \vec{x}_i and \vec{p}_i still are independent, and that for each $i \in \{1, \dots, N\}$, the probability law of each stochastic vector \vec{p}_i is the

same as in the absence of gravity, for the same value of b . Each stochastic vector \vec{x}_i is no more uniformly distributed in the vessel containing the gas: its probability density is higher at lower altitudes z , and this nonuniformity is more important for the heavier particles than for the lighter ones.

As in the previous section, the formulae given in 6.2.2 allow the calculation of $E(b)$ and $S(b)$. We observe that $E(b)$ now includes the potential energy of the gas in the gravity field, therefore should no more be called the internal energy of the gas.

6.3.3 Relativistic monoatomic ideal gas

In a Galilean reference frame, we consider a relativistic point particle of rest mass m , moving at a velocity \vec{v} . We denote by v the modulus of \vec{v} and by c the modulus of the velocity of light. The motion of the particle can be mathematically described by means of the Euler-Lagrange equations, with the Lagrangian

$$L = -mc^2 \sqrt{1 - \frac{v^2}{c^2}}.$$

The components of the linear momentum \vec{p} of the particle, in an orthonormal frame at rest in the considered Galilean reference frame, are

$$p_i = \frac{\partial L}{\partial v^i} = \frac{mv^i}{\sqrt{1 - \frac{v^2}{c^2}}}, \quad \text{therefore} \quad \vec{p} = \frac{m\vec{v}}{\sqrt{1 - \frac{v^2}{c^2}}}.$$

Denoting by p the modulus of \vec{p} , the Hamiltonian of the particle is

$$H = \vec{p} \cdot \vec{v} - L = \frac{mc^2}{\sqrt{1 - \frac{v^2}{c^2}}} = c\sqrt{p^2 + m^2c^2}.$$

Let us consider a relativistic gas, made of N point particles indexed by $i \in \{1, \dots, N\}$, m_i being the rest mass of the i -th particle. With the same assumptions as those made in Section 6.3.1, we can take for Hamiltonian of the gas

$$H = c \sum_{i=1}^N \sqrt{p_i^2 + m_i^2 c^2}.$$

With the same notations as those of Section 6.3.1, the partition function P of the gas takes the value, for each $b > 0$,

$$P(b) = \int_D \exp\left(-bc \sum_{i=1}^N \sqrt{(p_i)^2 + m_i^2 c^2}\right) \prod_{i=1}^N (d\vec{x}_i d\vec{p}_i).$$

This integral can be expressed in terms of the Bessel function K_2 , whose expression is, for each $x > 0$,

$$K_2(x) = x \int_0^{+\infty} \exp(-x \operatorname{ch} \chi) \operatorname{sh}^2 \chi \operatorname{ch} \chi d\chi.$$

We have

$$P(b) = \left(\frac{4\pi V c}{b} \right)^N \prod_{i=1}^N (m_i^2 K_2(m_i b c^2)),$$

$$\rho_b = \frac{1}{P(b)} \exp \left(-bc \sum_{i=1}^N \sqrt{p_i^2 + m_i^2 c^2} \right).$$

This probability density of the Gibbs state shows that the $2N$ stochastic vectors \vec{x}_i and \vec{p}_i are independent, that each \vec{x}_i is uniformly distributed in the vessel containing the gas and that the probability density of each \vec{p}_i is exactly the probability distribution of the linear momentum of particles in a relativistic gas called the *Maxwell-Jüttner distribution*, obtained by Ferencz Jüttner (1878–1958) in 1911, discussed in the book by the Irish mathematician and physicist J. L. Synge [60].

Of course, the formulae given in 6.2.2 allow the calculation of the internal energy $E(b)$, the entropy $S(b)$ and the pressure $\Pi(b)$ of the relativistic gas.

6.3.4 Relativistic ideal gas of massless particles

We have seen in the previous chapter that in an inertial reference frame, the Hamiltonian of a relativistic point particle of rest mass m is $c\sqrt{p^2 + m^2 c^2}$, where p is the modulus of the linear momentum vector \vec{p} of the particle in the considered reference frame. This expression still has a meaning when the rest mass m of the particle is 0. In an orthonormal reference frame, the equations of motion of a particle whose motion is mathematically described by a Hamiltonian system with Hamiltonian

$$H = cp = c\sqrt{p_1^2 + p_2^2 + p_3^2}$$

are

$$\begin{cases} \frac{dx^i}{dt} = \frac{\partial H}{\partial p_i} = c \frac{p_i}{p} \\ \frac{dp_i}{dt} = -\frac{\partial H}{\partial x^i} = 0, \end{cases} \quad (1 \leq i \leq 3),$$

which shows that the particle moves on a straight line at the velocity of light c . It seems therefore reasonable to describe a gas of N photons in a vessel of volume V at rest in an inertial reference frame by a Hamiltonian system, with the Hamiltonian

$$H = c \sum_{i=1}^N \|\vec{p}_i\| = c \sum_{i=1}^N \sqrt{p_{i1}^2 + p_{i2}^2 + p_{i3}^2}.$$

With the same notations as those used in the previous section, the partition function P of the gas takes the value, for each $b > 0$,

$$P(b) = \int_D \exp \left(-bc \sum_{i=1}^N \|\vec{p}_i\| \right) \prod_{i=1}^N (d\vec{x}_i d\vec{p}_i) = \left(\frac{8\pi V}{c^3 b^3} \right)^N.$$

The probability density of the corresponding Gibbs state, with respect to the Liouville measure $\lambda_\omega = \prod_{i=1}^N (d\vec{x}_i d\vec{p}_i)$, is

$$\rho_b = \prod_{i=1}^N \left(\frac{c^3 b^3}{8\pi V} \right) \exp(-bc \|\vec{p}_i\|).$$

This formula appears in the books by Sygne [60] and Souriau [55]. Physicists consider it as not adequate for the description of a gas of photons contained in a vessel at thermal equilibrium because the number of photons in the vessel, at any given temperature, cannot be imposed: it results from the processes of absorption and emission of photons by the walls of the vessel, heated at the imposed temperature, which spontaneously occur. In other words, this number is a stochastic function whose probability law is imposed by Nature. Souriau proposes, in his book [55], a way to account for the possible variation of the number of photons. Instead of using the *phase space* of the system of N massless relativistic particles contained in a vessel, he uses the *manifold of motions* M_N of that system (which is symplectomorphic to its phase space). He considers that the manifold of motions M of a system of photons in the vessel is the disjoint union

$$M = \bigcup_{N \in \mathbb{N}} M_N,$$

of all the manifolds of motions M_N of a system of N massless relativistic particles in the vessel, for all possible values of $N \in \mathbb{N}$. For $N = 0$ the manifold M_0 is reduced to a singleton with, as Liouville measure, the measure which takes the value 1 on the only non empty part of that manifold (the whole manifold M_0). Moreover, since any photon cannot be distinguished from any other photon, two motions of the system with the same number N of massless particles which only differ by the labelling of these particles must be considered as identical. Souriau considers too that since the number N of photons freely adjusts itself, the value of the parameter $b = \frac{1}{kT}$ must, at thermodynamic equilibrium, be the same in all parts M_N of the system, $N \in \mathbb{N}$. He uses too the fact that a photon can have two different states of (circular) polarization. With these assumptions the value at any b of the partition function of the system is

$$P(b) = \sum_{N=0}^{+\infty} \frac{1}{N!} \left(\frac{16\pi V}{c^3 b^3} \right)^N = \exp \left(\frac{16\pi V}{c^3 b^3} \right).$$

The number N of photons in the vessel at thermodynamic equilibrium is a stochastic function which takes the value n with the probability

$$\text{Probability}([N = n]) = \frac{1}{n!} \left(\frac{16\pi V}{c^3 b^3} \right)^n \exp \left(-\frac{16\pi V}{c^3 b^3} \right).$$

The expression of the partition function P allows the calculation of the internal energy, the entropy and all other thermodynamic functions of the system. However, the formula so obtained for the distribution of photons of various energies at a given temperature does not agree with the law, in very good agreement with experiments, obtained by Max Planck (1858–1947) in 1900. An assembly of photons in thermodynamic equilibrium evidently cannot be described as a classical Hamiltonian system. This fact played an important part for the development of Quantum Mechanics.

6.3.5 Specific heat of solids

The motion of a one-dimensional harmonic oscillator can be described by a Hamiltonian system with, as Hamiltonian,

$$H(p, q) = \frac{p^2}{2m} + \frac{\mu q^2}{2}.$$

The idea that the heat energy of a solid comes from the small vibrations, at a microscopic scale, of its constitutive atoms, lead physicists to attempt to mathematically describe a solid as an assembly of a large number N of three-dimensional harmonic oscillators. By dealing separately with each proper oscillation mode, the solid can even be described as an assembly of $3N$ one-dimensional harmonic oscillators. Exchanges of energy between these oscillators is allowed by the existence of small couplings between them. However, for the determination of the thermodynamic equilibria of the solid we will, as in the previous section for ideal gases, consider as negligible the energy of interactions between the oscillators. We therefore take for Hamiltonian of the solid

$$H = \sum_{i=1}^{3N} \left(\frac{p_i^2}{2m_i} + \frac{\mu_i q_i^2}{2} \right).$$

The value of the partition function P , for any $b > 0$, is

$$P(b) = \int_{\mathbb{R}^{6N}} \exp \left[-b \sum_{i=1}^{3N} \left(\frac{p_i^2}{2m_i} + \frac{\mu_i q_i^2}{2} \right) \right] \prod_{i=1}^{3N} (dp_i dq_i) = \prod_{i=1}^{3N} \left(\frac{1}{v_i} \right) b^{-3N},$$

where

$$v_i = \frac{1}{2\pi} \sqrt{\frac{\mu_i}{m_i}}$$

is the frequency of the i -th harmonic oscillator.

The internal energy of the solid is

$$E(b) = -\frac{d \log P(b)}{db} = \frac{3N}{b}.$$

We observe that it only depends on the the temperature and on the number of atoms in the solid, not on the frequencies v_i of the harmonic oscillators. With $b = \frac{1}{kT}$ this result is in agreement with the empirical law for the specific heat of solids discovered in 1819 by the French scientists Pierre Louis Dulong (1785–1838) and Alexis Thérèse Petit (1791–1820). This law is in good agreement with experiments at high temperature only. That fact was an important argument for a treatment of the specific heat of solids in the framework of Quantum Mechanics.

7 Generalization for Hamiltonian actions

7.1 Generalized Gibbs states

In his book [56] and in several papers [54, 57, 58], J.-M. Souriau extends the concept of a Gibbs state for a Hamiltonian action of a Lie group G on a symplectic manifold (M, ω) . Usual Gibbs states defined in section 6 for a smooth Hamiltonian H on a symplectic manifold (M, ω) appear as special cases, in which the Lie group is a one-parameter group. If the symplectic manifold (M, ω) is the *phase space* of the Hamiltonian system, that one-parameter group, whose parameter is the time t , is the group of evolution, as a function of time, of the state of the system, starting from its state at some arbitrarily chosen initial time t_0 . If (M, ω) is the symplectic manifold of all the *motions* of the system, that one-parameter group, whose parameter is a real $\tau \in \mathbb{R}$, is the transformation group which maps one motion of the system with some initial state at time t_0 onto the motion of the system with the same initial state at another time $(t_0 + \tau)$. We discuss below this generalization.

7.1.1 Notations and conventions

In this section, $\Phi : G \times M \rightarrow M$ is a Hamiltonian action (for example on the left) of a Lie group G on a symplectic manifold (M, ω) . We denote by \mathfrak{G} the Lie algebra of G , by \mathfrak{G}^* its dual space and by $J : M \rightarrow \mathfrak{G}^*$ a momentum map of the action Φ .

7.1.2 Definitions. A *generalized temperature* is an element $b \in \mathfrak{G}$ such that the integral in the right hand side of the equality

$$P(b) = \int_M \exp(-\langle J, b \rangle) d\lambda_\omega$$

is *normally convergent*, which means that there exists an open neighbourhood U in \mathfrak{G} and a positive-valued function $f : M \rightarrow \mathbb{R}^+$, integrable on M with respect to the Liouville measure λ_ω , satisfying, for any $b' \in U$, $\exp(-\langle J, b' \rangle) \leq f$.

The *partition function* associated to the momentum map J is the function P , defined on the set Ω of generalized temperatures, with values in \mathbb{R}^+ , which associates to each $b \in \Omega$ the real $P(b)$ defined by the above equality.

The *generalized Gibbs state* associated to a generalized temperature $b \in \Omega$ is the probability measure on M with density, with respect to the Liouville measure λ_ω ,

$$\rho_b = \frac{1}{P(b)} \exp(-\langle J, b \rangle).$$

7.1.3 Proposition. *With the notations and assumptions of 7.1.1 and 7.1.2, let us assume in addition that the set Ω of generalized temperatures is not empty. Then Ω is a convex open subset of \mathfrak{G} which does not depend on the choice of the momentum map J , and the partition function $P : \Omega \rightarrow \mathbb{R}^+$ is a differentiable function of class C^∞ whose differentials of all orders can be calculated by differentiations with respect to generalized temperature b of the integral expressing $P(b)$, under the integration sign \int_M .*

Proof. Let us follow the proof given by Souriau in [56]. Definitions 7.1.2 prove that when $b \in \mathfrak{G}$ is a generalized temperature, there exists an open neighbourhood U of b all of whose elements are generalized temperatures. The set Ω of generalized temperatures is therefore an open subset of \mathfrak{G} . If we replace the momentum map J by $J + \mu$, where μ is a constant element in \mathfrak{G}^* , the function $\exp(-\langle J, b \rangle)$ is replaced by $\exp(-\langle \mu, b \rangle) \exp(-\langle J, b \rangle)$, which is normally integrable on M if and only if the function $\exp(-\langle J, b \rangle)$ itself is normally integrable on M . Therefore the set Ω does not depend on the choice of J .

Let b_0 and b_1 be two distinct elements in Ω , U_0 and U_1 be open neighbourhoods, respectively of b_0 and of b_1 , f_0 and f_1 be positive valued functions defined on M , integrable with respect to the Liouville measure λ_ω , satisfying $\exp(-\langle J, b'_0 \rangle) \leq f_0$ and $\exp(-\langle J, b'_1 \rangle) \leq f_1$ for any $b'_0 \in U_0$ and $b'_1 \in U_1$. For any $\lambda \in [0, 1]$, $U_\lambda = \{(1 - \lambda)b'_0 + \lambda b'_1 \mid b'_0 \in U_0, b'_1 \in U_1\}$ is an open neighbourhood of $b_\lambda = (1 - \lambda)b_0 + \lambda b_1$, the function $f_\lambda = (1 - \lambda)f_0 + \lambda f_1$ is integrable on M with respect to the Liouville measure and satisfies, for each $b'_\lambda \in U_\lambda$, $\exp(-\langle J, b'_\lambda \rangle) \leq f_\lambda$. Therefore $b_\lambda \in \Omega$, which proves that Ω is convex.

The k -th differential of $\exp(-\langle J, b \rangle)$ with respect to b is

$$D^k \left(\exp(-\langle J, b \rangle) \right) = (-1)^k J^{\otimes k} \exp(-\langle J, b \rangle).$$

Let us choose a norm on \mathfrak{G} . We define a norm on the space $\mathcal{L}^k(\mathfrak{G}, \mathbb{R})$ of k -multilinear forms on \mathfrak{G} by setting, for each $\xi \in \mathcal{L}^k(\mathfrak{G}, \mathbb{R})$,

$$\|\xi\| = \sup_{X_i \in \mathfrak{G}, \|X_i\|=1, 1 \leq i \leq k} |\xi(X_1, \dots, X_k)|.$$

Let $b \in \Omega$ be a generalized temperature, $\varepsilon > 0$ be a constant and f be a positive valued function integrable on M with respect to the measure λ_ω which satisfies $\exp(-\langle J, b' \rangle) \leq f$ for any $b' \in \mathcal{G}$ such that $\|b' - b\| \leq \varepsilon$. Let $b'' \in \mathcal{G}$ satisfying $\|b'' - b\| \leq \frac{\varepsilon}{2}$. For any $X \in \mathcal{G}$ satisfying $\|X\| = 1$,

$$|\langle J, X \rangle| \leq \frac{2k}{\varepsilon} \exp\left(\frac{\varepsilon}{2k} |\langle J, X \rangle|\right),$$

therefore

$$|\langle J, X \rangle|^k \exp(-\langle J, b'' \rangle) \leq \left(\frac{2k}{\varepsilon}\right)^k \exp\left(-\langle J, b'' \pm \frac{\varepsilon}{2} X \rangle\right),$$

where the sign \pm is chosen in such a way that $-\langle J, \pm \varepsilon X \rangle \geq 0$. Since $\|b - b'' \pm \frac{\varepsilon}{2} X\| \leq \varepsilon$, we have

$$\left\| D^k \left(\exp(-\langle J, b'' \rangle) \right) \right\| \leq \frac{2k}{\varepsilon} f,$$

which proves that for any integer $k > 0$ the k -th differential, with respect to b , of the function $\exp(-\langle J, b \rangle)$ is normally integrable on M with respect to the Liouville measure λ_ω . The partition function P is therefore of class C^∞ on Ω , and its differentials of all orders can be calculated by differentiation under the integration sign \int_M . \square

The following Proposition generalizes 6.1.11.

7.1.4 Proposition. *Assumptions and notations are the same as in 7.1.3. Let $b \in \Omega$ be a generalized temperature. The integral in the right hand side of the below equality, which defines the mean value of the momentum J for the generalized Gibbs state associated to b ,*

$$\mathcal{E}_{\rho_b}(J) = \frac{1}{P(b)} \int_M J \exp(-\langle J, b \rangle) d\lambda_\omega$$

converges. For any other probability density ρ_1 such that $\mathcal{E}_{\rho_1}(J) = \mathcal{E}_{\rho_b}(J)$, we have

$$s(\rho_1) \leq s(\rho_b),$$

and the equality $s(\rho_1) = s(\rho_b)$ holds if and only if $\rho_1 = \rho_b$.

Proof. The convergence of the integral defining $\mathcal{E}_{\rho_b}(J)$ follows from 7.1.3. The remaining of the proof is the same as that of Proposition 6.1.11. \square

7.1.5 Proposition. *Assumptions and notations are the same as in 7.1.3. Let $b \in \Omega$ be a generalized temperature. The generalized Gibbs state associated to b remains invariant under the restriction of the Hamiltonian action Φ to the one-parameter subgroup of G generated by b , $\{\exp(\tau b) \mid \tau \in \mathbb{R}\}$.*

Proof. The orbits of the action on M of the subgroup $\{\exp(\tau b) \mid \tau \in \mathbb{R}\}$ of G are the integral curves of the Hamiltonian vector field whose Hamiltonian is $\langle J, b \rangle$, which of course is constant on each of these curves. Therefore the proof of 6.1.12 is valid for that subgroup. \square

7.2 Generalized thermodynamic functions

7.2.1 Proposition. *Let $\Phi : G \times M \rightarrow M$ be a Hamiltonian action of a Lie group G on a symplectic manifold (M, ω) , such that the set Ω of generalized temperatures (7.1.2) is not empty. For each generalized temperature $b \in \Omega$, let*

$$E_J(b) = \mathcal{E}_{\rho_b}(J) = \frac{1}{P(b)} \int_M J \exp(-\langle J, b \rangle) d\lambda_\omega,$$

$$S(b) = s(\rho_b) = \int_M \rho_b \log \left(\frac{1}{\rho_b} \right) d\lambda_\omega,$$

where ρ_b is the probability density of the generalized Gibbs state associated to b (7.1.2). The functions $E_J : \Omega \rightarrow \mathcal{G}^*$ and $S : \Omega \rightarrow \mathbb{R}$ so defined, called, respectively, the mean value of J and the entropy in the generalized Gibbs state associated to b , are differentiable of class C^∞ and can be expressed in terms of the partition function $P : \Omega \rightarrow \mathbb{R}^+$ or its logarithm $\log P : \Omega \rightarrow \mathbb{R}$ and their differentials (7.1.2) as follows,

$$E_J(b) = -\frac{1}{P(b)} DP(b) = -D(\log P)(b),$$

$$S(b) = (\log P)(b) + \langle E_J(b), b \rangle = (\log P)(b) - \langle D(\log P)(b), b \rangle.$$

For each $b \in \Omega$, the differential at b of the map E_J (which is a linear map defined on \mathcal{G} , with values in its dual \mathcal{G}^*) is given by

$$\langle DE_J(b)(Y), Z \rangle = \langle E_J(b), Y \rangle \langle E_J(b), Z \rangle - \mathcal{E}_{\rho_b}(\langle J, Y \rangle \langle J, Z \rangle), \quad \text{with } Y \text{ and } Z \in \mathcal{G},$$

where we have written, as in 6.1.8,

$$\mathcal{E}_{\rho_b}(\langle J, Y \rangle \langle J, Z \rangle) = \frac{1}{P(b)} \int_M \langle J, Y \rangle \langle J, Z \rangle \exp(-\langle J, b \rangle) d\lambda_\omega.$$

At each $b \in \Omega$, the differential of the entropy function S (7.1.4), which is a linear map defined on \mathcal{G} , with values in \mathbb{R} , in other words an element of \mathcal{G}^* , is given by

$$\langle DS(b), Y \rangle = \langle DE_J(b)(Y), b \rangle, \quad Y \in \mathcal{G}.$$

Proof. Proposition 7.1.3 asserts that the partition function P is of class C^∞ and that its differentials of all orders can be calculated by differentiation under the integration sign \int_M . The expressions of E_J and S easily follow, show that these functions are of class C^∞ and easily allow the determination of their differentials. \square

7.2.2 Corollary. *With the same assumptions and notations as those in Proposition 7.2.1, for any $b \in \Omega$ and $Y \in \mathcal{G}$,*

$$\langle DE_J(b)(Y), Y \rangle = -\frac{1}{P(b)} \int_M \langle J - E_J(b), Y \rangle^2 \exp(-\langle J, b \rangle) d\lambda_\omega.$$

We always have $\langle DE_J(b)(Y), Y \rangle \leq 0$, and when $\langle J, Y \rangle$ is not a constant function on M , i.e., when the subgroup of G generated by the flow of the Hamiltonian vector field with $\langle J, Y \rangle$ as Hamiltonian acts effectively on the symplectic manifold (M, ω) , we have $\langle DE_J(b)(Y), Y \rangle < 0$.

Proof. The above equality follows from the well known result in Probability theory already used in the proof of 6.2.2. We observe that $\langle DE_J(b)(Y), Y \rangle$ is the opposite of the square of the standard deviation of the stochastic variable $\langle J, Y \rangle$, for the probability measure of density ρ_b on M with respect to the Liouville measure λ_ω , i.e., for the generalized Gibbs state associated to b . That quantity is therefore always ≤ 0 , and is equal to 0 if and only if $\langle J, Y \rangle$ is a constant function on M . \square

7.2.3 Theorem. *With the same assumptions and notations as those in Proposition 7.2.1, we assume in addition that the Hamiltonian action Φ of the Lie group G on the symplectic manifold (M, ω) is effective, i.e., such that for any $X \in \mathfrak{g} \setminus \{0\}$ the function $\langle J, X \rangle$ is not constant on M . The map E_J then is a diffeomorphism of the open subset of generalized temperatures $\Omega \subset \mathfrak{g}$ onto an open subset $\Omega^* \subset \mathfrak{g}^*$.*

Proof. Since, by 7.2.2, for each $b \in \Omega$ and $Y \in \mathfrak{g} \setminus \{0\}$ we have $\langle DE_J(b)(Y), Y \rangle < 0$, for any $b \in \Omega$ the differential DE_J of E_J is invertible. The map E_J , which is known to be differentiable of class C^∞ , is therefore open. To prove that this map is a diffeomorphism onto an open subset of \mathfrak{g}^* , it is enough to prove that it is injective. Let us assume that there exists two elements b_0 and $b_1 \in \Omega$, $b_1 - b_0 \neq 0$, such that $E_J(b_1) = E_J(b_0)$. Since Ω is convex (7.1.3), $b(\lambda) = (1 - \lambda)b_0 + \lambda b_1 \in \Omega$ for any $\lambda \in [0, 1]$, and we have

$$0 = \langle E_J(b_1) - E_J(b_0), b_1 - b_0 \rangle = \int_0^1 \langle DE_J(b(\lambda))(b_1 - b_0), b_1 - b_0 \rangle d\lambda.$$

The integrated function in the right hand side of this double equality is continuous and by 7.2.2 its values are everywhere < 0 on $[0, 1]$. Its integral therefore cannot be equal to 0. We have proven that $E_J(b_1)$ cannot be equal to $E_J(b_0)$. The map E_J therefore is injective. \square

7.2.4 Remarks.

1. With the assumptions of 7.2.3 since, for any $b \in \Omega$, $E_J(b) = -D(\log P)(b)$, we have, for any $Y \in \mathfrak{g} \setminus \{0\}$

$$D^2(\log P)(b)(Y, Y) = -\langle DE_J(b)(Y), Y \rangle > 0.$$

The second differential of $\log P$ therefore is, at each $b \in \Omega$, a symmetric definite positive bilinear form. Frédéric Barbaresco [7] ha shown that it is linked to the *Fisher metric* which appers in Information theory.

2. The equality

$$S(b) = \langle D(-\log P)(b), b \rangle - (-\log P)(b)$$

expresses the fact that the functions $-\log P : \Omega \rightarrow \mathbb{R}$ and $S \circ E_J^{-1} : \Omega^* \rightarrow \mathbb{R}$ are *Legendre transforms* of each other: they are related by the same formula as that which relates, in Calculus of variations on a smooth manifold N , an hyper-regular Lagrangian $L : TN \rightarrow \mathbb{R}$ and the associated Hamiltonian $H : T^*N \rightarrow \mathbb{R}$. In that setting the Legendre map $\mathcal{L}_L : TN \rightarrow T^*N$ is the vertical differential of the Lagrangian L , and its inverse is the vertical differential of the Hamiltonian. Here the Legendre map is $E_J : \Omega \rightarrow \Omega^*$, equal to the differential $D(-\log P)$ of the function $-\log P$, which plays the part of the Lagrangian. Its inverse $E_J^{-1} : \Omega^* \rightarrow \Omega$ is equal to the differential $D(S \circ E_J^{-1})$ of the function $S \circ E_J^{-1}$, which plays the part of the Hamiltonian:

$$E_J = D(-\log P), \quad (E_J)^{-1} = D(S \circ E_J^{-1}).$$

Legendre transforms were used in Thermodynamics by the French scientist François Massieu in his very early works [40, 41], more systematically presented in [42], in which he introduced his *characteristic functions* (today called *thermodynamic potentials*) allowing the determination of all the thermodynamic functions of a physical system by partial derivations of a suitably chosen characteristic function. For a modern presentation of that subject the reader is referred to [4] and [11], chapter 5, pp. 131–152.

The momentum map J of the Hamiltonian action Φ is not uniquely determined: for any constant $\mu \in \mathfrak{G}^*$, $J_1 = J + \mu$ too is a momentum map for Φ . The following proposition indicates how the generalized thermodynamic functions P , E_J and S change when J is replaced by J_1 .

7.2.5 Proposition. *With the same assumptions and notations as those in Proposition 7.2.1, let $\mu \in \mathfrak{G}^*$ be a constant. When the momentum map J is replaced by $J_1 = J + \mu$, the open subset Ω of \mathfrak{G} remains unchanged, while the generalized thermodynamic functions P , E_J and S , are replaced, respectively, by P_1 , E_{J_1} and S_1 , given by*

$$P_1(b) = \exp(-\langle \mu, b \rangle) P(b), \quad E_{J_1}(b) = E_J(b) + \mu, \quad S_1(b) = S(b).$$

The Gibbs statistical state and its density ρ_b with respect to the Liouville measure λ_ω remain unchanged.

Proof. We have

$$\exp(-\langle J + \mu, b \rangle) = \exp(-\langle \mu, b \rangle) \exp(-\langle J, b \rangle).$$

The indicated results follow by easy calculations. \square

The following proposition indicates how the generalized thermodynamic functions P , E_J and S vary along orbits of the adjoint action of the Lie group G on its Lie algebra \mathfrak{G} .

7.2.6 Proposition. *The assumptions and notations are the same as those in Proposition 7.2.1. The open subset Ω of \mathfrak{G} is an union of orbits of the adjoint action of G on \mathfrak{G} . In other words, for each $b \in \Omega$ and each $g \in G$, $\text{Ad}_g b \in \Omega$. Moreover, let $\theta : G \rightarrow \mathfrak{G}^*$ be the symplectic cocycle of G for the coadjoint action of G on \mathfrak{G}^* such that, for any $g \in G$,*

$$J \circ \Phi_g = \text{Ad}_{g^{-1}}^* \circ J + \theta(g).$$

Then for each $b \in \Omega$ and each $g \in G$

$$\begin{aligned} P(\text{Ad}_g b) &= \exp(\langle \theta(g^{-1}), b \rangle) P(b) = \exp(-\langle \text{Ad}_g^* \theta(g), b \rangle) P(b), \\ E_J(\text{Ad}_g b) &= \text{Ad}_{g^{-1}}^* E_J(b) + \theta(g), \\ S(\text{Ad}_g b) &= S(b). \end{aligned}$$

Proof. We have

$$\begin{aligned} P(\text{Ad}_g b) &= \int_M \exp(-\langle J, \text{Ad}_g b \rangle) d\lambda_\omega = \int_M \exp(-\langle \text{Ad}_g^* J, b \rangle) d\lambda_\omega \\ &= \int_M \exp(-\langle J \circ \Phi_{g^{-1}} - \theta(g^{-1}), b \rangle) d\lambda_\omega \\ &= \exp(\langle \theta(g^{-1}), b \rangle) P(b) = \exp(-\langle \text{Ad}_g^* \theta(g), b \rangle) P(b), \end{aligned}$$

since $\theta(g^{-1}) = -\text{Ad}_g^* \theta(g)$. By using 7.2.1 and 7.1.4, the other results easily follow. \square

7.2.7 Remark. The equality

$$E_J(\text{Ad}_g b) = \text{Ad}_{g^{-1}}^* E_J(b) + \theta(g)$$

means that the map $E_J : \Omega \rightarrow \mathfrak{G}^*$ is equivariant with respect to the adjoint action of G on the open subset Ω of its Lie algebra \mathfrak{G} and its affine action on the left on \mathfrak{G}^*

$$(g, \xi) \mapsto \text{Ad}_{g^{-1}}^* \xi + \theta(g), \quad g \in G, \quad \xi \in \mathfrak{G}^*.$$

7.2.8 Proposition. *The assumptions and notations are the same as those in Proposition 7.2.1. For each $b \in \Omega$ and each $X \in \mathfrak{G}$, we have*

$$\begin{aligned} \langle E_J(b), [X, b] \rangle &= \langle \Theta(X), b \rangle, \\ DE_J(b)([X, b]) &= -\text{ad}_X^* E_J(b) + \Theta(X), \end{aligned}$$

where $\Theta = T_e \theta : \mathfrak{G} \rightarrow \mathfrak{G}^*$ is the 1-cocycle of the Lie algebra \mathfrak{G} associated to the 1-cocycle θ of the Lie group G .

Proof. Let us set $g = \exp(\tau X)$ in the first equality in 7.2.6, derive that equality with respect to τ , and evaluate the result at $\tau = 0$. We obtain

$$DP(b)([X, b]) = -P(b) \langle \Theta(X), b \rangle.$$

Since, by the first equality of 7.2.1, $DP(b) = -P(b)E_J(b)$, the first stated equality follows.

Let us now set $g = \exp(\tau X)$ in the second equality in 7.2.6, derive that equality with respect to τ , and evaluate the result at $\tau = 0$. We obtain the second equality stated. \square

7.2.9 Corollary. *With the assumptions and notations of 7.2.8, let us define, for each $b \in \Omega$, a linear map $\Theta_b : \mathfrak{G} \rightarrow \mathfrak{G}^*$ by setting*

$$\Theta_b(X) = \Theta(X) - \text{ad}_X^* E_J(b).$$

The map Θ_b is a symplectic 1-cocycle of the Lie algebra \mathfrak{G} for the coadjoint representation, which satisfies

$$\Theta_b(b) = 0.$$

Moreover if we replace the momentum map J by $J_1 = J + \mu$, with $\mu \in \mathfrak{G}^$ constant, the 1-cocycle Θ_b remains unchanged.*

Proof. For X, Y and Z in \mathfrak{G} , since Θ is a 1-cocycle, $\sum_{\text{circ}(X,Y,Z)}$ meaning a sum over circular permutations of X, Y and Z , using the Jacobi identity in \mathfrak{G} , we have

$$\begin{aligned} \sum_{\text{circ}(X,Y,Z)} \langle \Theta_b(X), [Y, Z] \rangle &= \sum_{\text{circ}(X,Y,Z)} \langle -\text{ad}_X^* E_J(b), [Y, Z] \rangle \\ &= \sum_{\text{circ}(X,Y,Z)} \langle -E_J(b), [X, [Y, Z]] \rangle \\ &= 0. \end{aligned}$$

The linear map Θ_b is therefore a 1-cocycle, even a symplectic 1-cocycle since for all X and $Y \in \mathfrak{G}$, $\langle \Theta_b(X), Y \rangle = -\langle \Theta_b(Y), X \rangle$.

Using the first equality stated in 7.2.8, we have for any $X \in \mathfrak{G}$

$$\langle \Theta_b(b), X \rangle = \langle \Theta(b) - \text{ad}_b^* E_J(b), X \rangle = -\langle \Theta(X), b \rangle + \langle E_J(b), [X, b] \rangle = 0.$$

If we replace J by $J_1 = J + \mu$, the map $X \mapsto \Theta(X)$ is replaced by $X \mapsto \Theta_1(X) = \Theta(X) + \text{ad}_X^* \mu$ and $E_J(b)$ by $E_{J_1}(b) = E_J(b) + \mu$, therefore Θ_b remains unchanged. \square

The following lemma will allow us to define, for each $b \in \Omega$, a remarkable symmetric bilinear form on the vector subspace $[b, \mathfrak{G}] = \{[b, X]; X \in \mathfrak{G}\}$ of the Lie algebra \mathfrak{G} .

7.2.10 Lemma. *Let Ξ be a 1-cocycle of a finite-dimensional Lie algebra \mathfrak{G} for the coadjoint representation. For each $b \in \ker \Xi$, let $F_b = [b, \mathfrak{G}]$ be the set of elements $X \in \mathfrak{G}$ which can be written $X = [X_1, b]$ for some $X_1 \in \mathfrak{G}$. Then F_b is a vector subspace of \mathfrak{G} , and the value of the right hand side of the equality*

$$\Gamma_b(X, Y) = \langle \Xi(X_1), Y \rangle, \quad \text{with } X_1 \in \mathfrak{G}, X = [X_1, b] \in F_b, Y \in F_b,$$

depends only on X and Y , not on the choice of $X_1 \in \mathfrak{G}$ such that $X = [X_1, b]$. That equality defines a bilinear form Γ_b on F_b which is symmetric, i.e. satisfies

$$\Gamma_b(X, Y) = \Gamma_b(Y, X) \quad \text{for all } X \text{ and } Y \in F_b.$$

Proof. Let X_1 and $X'_1 \in \mathfrak{G}$ be such that $[X_1, b] = [X'_1, b] = X$. Let $Y_1 \in \mathfrak{G}$ be such that $[Y_1, b] = Y$. We have

$$\begin{aligned} \langle \Xi(X_1 - X'_1), Y \rangle &= \langle \Xi(X_1 - X'_1), [Y_1, b] \rangle \\ &= -\langle \Xi(Y_1), [b, X_1 - X'_1] \rangle - \langle \Xi(b), [X_1 - X'_1, Y_1] \rangle \\ &= 0 \end{aligned}$$

since $\Xi(b) = 0$ and $[b, X_1 - X'_1] = 0$. We have shown that $\langle \Xi(X_1), Y \rangle = \langle \Xi(X'_1), Y \rangle$. Therefore Γ_b is a bilinear form on F_b . Similarly

$$\langle \Xi(X_1), Y \rangle = \langle \Xi(X_1), [Y_1, b] \rangle = -\langle \Xi(Y_1), [b, X_1] \rangle - \langle \Xi(b), [X_1, Y_1] \rangle = \langle \Xi(Y_1), X \rangle,$$

which proves that Γ_b is symmetric. \square

7.2.11 Theorem. *The assumptions and notations are the same as those in Proposition 7.2.1. For each $b \in \Omega$, there exists on the vector subspace $F_b = [b, \mathfrak{G}]$ of elements $X \in \mathfrak{G}$ which can be written $X = [X_1, b]$ for some $X_1 \in \mathfrak{G}$, a symmetric negative bilinear form Γ_b given by*

$$\Gamma_b(X, Y) = \langle \Theta_b(X_1), Y \rangle, \quad \text{with } X_1 \in \mathfrak{G}, X = [X_1, b] \in F_b, Y \in F_b,$$

where $\Theta_b : \mathfrak{G} \rightarrow \mathfrak{G}^*$ is the symplectic 1-cocycle defined in 7.2.9.

Proof. We have seen in 7.2.9 that $b \in \ker \Theta_b$. The fact that the equality given in the statement above defines indeed a symmetric bilinear form on F_b directly follows from Lemma 7.2.10. We only have to prove that this symmetric bilinear form is negative. Let $X \in F_b$ and $X_1 \in \mathfrak{G}$ such that $X = [X_1, b]$. Using 7.2.8 and 7.2.2, we have

$$\begin{aligned} \Gamma_b(X, X) &= \langle \Theta_b(X_1), [X_1, b] \rangle = \langle \Theta(X_1) - \text{ad}_{X_1}^* E_J(b), [X_1, b] \rangle = \langle DE_J(b)[X_1, b], [X_1, b] \rangle \\ &\leq 0. \end{aligned}$$

The symmetric bilinear form Γ_b on F_b is therefore negative. \square

7.2.12 Remarks. Let $b \in \Omega$ be a generalized temperature.

1. The symmetric negative bilinear form Γ_b defined in 7.2.11 is the restriction to the vector subspace F_b of \mathfrak{G} of the opposite of the symmetric positive bilinear form on \mathfrak{G} defined in 7.2.2. We have seen that when the action Φ of the Lie group G on the symplectic manifold (M, ω) is effective, that form is non-degenerate.

2. The vector subspace F_b of \mathfrak{G} made by elements $X \in \mathfrak{G}$ which can be written as $X = [X_1, b]$, with $X_1 \in \mathfrak{G}$, has a very simple geometric interpretation: it is the set of directions tangent at b to the adjoint orbit of that point. Therefore when the action Φ is effective, the bilinear forms $-\Gamma_b$, for all elements b of an adjoint orbit contained in Ω , determine a Riemannian metric on that orbit.

7.3 Examples of generalized Gibbs states

7.3.1 Action of the group of rotations on a sphere

The symplectic manifold (M, ω) considered here is the two-dimensional sphere of radius R centered at the origin O of a three-dimensional oriented Euclidean vector space \vec{E} , equipped with its area element as symplectic form. The group G of rotations around the origin (isomorphic to $\text{SO}(3)$) acts on the sphere M by a Hamiltonian action. The Lie algebra \mathfrak{G} of G can be identified with \vec{E} , the fundamental vector field on M associated to an element \vec{b} in $\mathfrak{G} \equiv \vec{E}$ being the vector field on M whose value at a point $m \in M$ is given by the vector product $\vec{b} \times \vec{Om}$. The dual \mathfrak{G}^* of \mathfrak{G} will be too identified with \vec{E} , the coupling by duality being given by the Euclidean scalar product. The momentum map $J : M \rightarrow \mathfrak{G}^* \equiv \vec{E}$ is given by

$$J(m) = -R\vec{Om}, \quad m \in M.$$

Therefore, for any $\vec{b} \in \mathfrak{G} \equiv \vec{E}$,

$$\langle J(m), \vec{b} \rangle = -R\vec{Om} \cdot \vec{b}.$$

Let \vec{b} be any element in $\mathfrak{G} \equiv \vec{E}$. To calculate the partition function $P(\vec{b})$ we choose an orthonormal basis $(\vec{e}_x, \vec{e}_y, \vec{e}_z)$ of \vec{E} such that $\vec{b} = \|\vec{b}\| \vec{e}_z$, with $\|\vec{b}\| \in \mathbb{R}^+$, and we use angular coordinates (φ, θ) on the sphere M . The coordinates of a point $m \in M$ are

$$x = R \cos \theta \cos \varphi, \quad y = R \cos \theta \sin \varphi, \quad z = R \sin \theta.$$

We have

$$P(\vec{b}) = \int_0^{2\pi} \left(\int_{-\pi/2}^{\pi/2} R^2 \exp(R\|\vec{b}\| \sin \theta) d\theta \right) d\varphi = \frac{4\pi R}{\|\vec{b}\|} \text{sh}(R\|\vec{b}\|).$$

The probability density (with respect to the natural area measure on the sphere M) of the generalized Gibbs state associated to \vec{b} is

$$\rho_b(m) = \frac{1}{P(\vec{b})} \exp(\vec{Om} \cdot \vec{b}), \quad m \in M.$$

We observe that ρ_b reaches its maximal value at the point $m \in M$ such that $\vec{Om} = \frac{R\vec{b}}{\|\vec{b}\|}$ and its minimal value at the diametrically opposed point.

7.3.2 The Galilean group, its Lie algebra and its actions

In view of the presentation, made below, of some physically meaningful generalized Gibbs states for Hamiltonian actions of subgroups of the Galilean group, we recall in this section some notions about the space-time of classical (non-relativistic) Mechanics, the Galilean group, its Lie algebra and its Hamiltonian actions. The interested reader will find a much more detailed treatment on these subjects in the book by Souriau [55] or in the recent book by G. de Saxcé and C. Vallée [52]. The paper [51] presents a nice application of Galilean invariance in Thermodynamics.

The space-time of classical Mechanics is a four-dimensional real affine space which, once an inertial reference frame, units of length and time, orthonormal bases of space and time are chosen, can be identified with $\mathbb{R}^4 \equiv \mathbb{R}^3 \times \mathbb{R}$ (coordinates x, y, z, t). The first three coordinates x, y and z can be considered as the three components of a vector $\vec{r} \in \mathbb{R}^3$, therefore an element of space-time can be denoted by (\vec{r}, t) . However, as the action of the Galilean group will show, the splitting of space-time into space and time is not uniquely determined, it depends on the choice of an inertial reference frame. In classical Mechanics, there exists an absolute time, but no absolute space. There exists instead a space (which is an Euclidean affine three-dimensional space) for each value of the time. The spaces for two distinct values of the time should be considered as disjoint.

The space-time being identified with $\mathbb{R}^3 \times \mathbb{R}$ as explained above, the Galilean group G can be identified with the set of matrices of the form

$$\begin{pmatrix} A & \vec{b} & \vec{d} \\ 0 & 1 & e \\ 0 & 0 & 1 \end{pmatrix}, \quad \text{with } A \in \text{SO}(3), \vec{b} \text{ and } \vec{d} \in \mathbb{R}^3, e \in \mathbb{R}, \quad (*)$$

the vector space \mathbb{R}^3 being oriented and endowed with its usual Euclidean structure, the matrix $A \in \text{SO}(3)$ acting on it.

The action of the Galilean group G on space-time, identified as indicated above with $\mathbb{R}^3 \times \mathbb{R}$, is the affine action

$$\begin{pmatrix} \vec{r} \\ t \\ 1 \end{pmatrix} \mapsto \begin{pmatrix} A & \vec{b} & \vec{d} \\ 0 & 1 & e \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \vec{r} \\ t \\ 1 \end{pmatrix} = \begin{pmatrix} A\vec{r} + t\vec{b} + \vec{d} \\ t + e \\ 1 \end{pmatrix}.$$

The Lie algebra \mathfrak{G} of the Galilean group G can be identified with the space of matrices of the form

$$\begin{pmatrix} j(\vec{\omega}) & \vec{\beta} & \vec{\delta} \\ 0 & 0 & \varepsilon \\ 0 & 0 & 0 \end{pmatrix}, \quad \text{with } \vec{\omega}, \vec{\beta} \text{ and } \vec{\delta} \in \mathbb{R}^3, \varepsilon \in \mathbb{R}. \quad (**)$$

We have denoted by $j(\vec{\omega})$ the 3×3 skew-symmetric matrix

$$j(\vec{\omega}) = \begin{pmatrix} 0 & -\omega_z & \omega_y \\ \omega_z & 0 & -\omega_x \\ -\omega_y & \omega_x & 0 \end{pmatrix}.$$

The matrix $j(\vec{\omega})$ is an element in the Lie algebra $\mathfrak{so}(3)$, and its action on a vector $\vec{r} \in \mathbb{R}^3$ is given by the vector product

$$j(\vec{\omega})\vec{r} = \vec{\omega} \times \vec{r}.$$

Let us consider a mechanical system made by a point particle of mass m whose position and velocity at time t , in the reference frame allowing the identification of space-time with $\mathbb{R}^3 \times \mathbb{R}$, are the vectors \vec{r} and $\vec{v} \in \mathbb{R}^3$. The action of an element of the Galilean group on \vec{r}, \vec{v} and t can be written as

$$\begin{pmatrix} \vec{r} & \vec{v} \\ t & 1 \\ 1 & 0 \end{pmatrix} \mapsto \begin{pmatrix} A & \vec{b} & \vec{d} \\ 0 & 1 & e \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \vec{r} & \vec{v} \\ t & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} A\vec{r} + t\vec{b} + \vec{d} & A\vec{v} + \vec{b} \\ t + e & 1 \\ 1 & 0 \end{pmatrix}.$$

Souriau has shown in his book [55] that this action is Hamiltonian, with the map J , defined on the evolution space of the particle, with value in the dual \mathcal{G}^* of the Lie algebra \mathcal{G} of the Galilean group, as momentum map

$$J(\vec{r}, t, \vec{v}, m) = m \left(\vec{r} \times \vec{v}, \vec{r} - t\vec{v}, \vec{v}, \frac{1}{2}\|\vec{v}\|^2 \right).$$

Let $b = \begin{pmatrix} j(\vec{\omega}) & \vec{\beta} & \vec{\delta} \\ 0 & 0 & \varepsilon \\ 0 & 0 & 0 \end{pmatrix}$ be an element in \mathcal{G} . Its coupling with $J(\vec{r}, t, \vec{v}, m) \in \mathcal{G}^*$ is given by the formula

$$\langle J(\vec{r}, t, \vec{v}, m), b \rangle = m \left(\vec{\omega} \cdot (\vec{r} \times \vec{v}) - (\vec{r} - t\vec{v}) \cdot \vec{\beta} + \vec{v} \cdot \vec{\delta} - \frac{1}{2}\|\vec{v}\|^2 \varepsilon \right).$$

7.3.3 One-parameter subgroups of the Galilean group

In his book [55], J.-M. Souriau has shown that when the Lie group action Φ is the action of the full Galilean group on the space of motions of an isolated mechanical system, the open subset Ω of the Lie algebra \mathcal{G} of the Galilean group made by generalized temperatures (7.1.2) is empty. In other words, generalized Gibbs states of the full Galilean group do not exist. However, generalized Gibbs states for one-parameter subgroups of the Galilean group do exist which have an interesting physical meaning.

Let us consider the element b of \mathcal{G} given by formula (*) of 7.3.2, and assume that $\varepsilon \neq 0$. The one-parameter subgroup G_1 of the Galilean group generated by b is the set of matrices $\exp(\tau b)$, with $\tau \in \mathbb{R}$. We have

$$\exp(\tau b) = \begin{pmatrix} A(\tau) & \vec{b}(\tau) & \vec{d}(\tau) \\ 0 & 1 & \tau\varepsilon \\ 0 & 0 & 1 \end{pmatrix},$$

with

$$\begin{aligned} A(\tau) &= \exp(\tau j(\vec{\omega})), \\ \vec{b}(\tau) &= \left(\sum_{n=1}^{\infty} \frac{\tau^n}{n!} (j(\vec{\omega}))^{n-1} \right) \vec{\beta}, \\ \vec{d}(\tau) &= \left(\sum_{n=1}^{\infty} \frac{\tau^n}{n!} (j(\vec{\omega}))^{n-1} \right) \vec{\delta} + \varepsilon \left(\sum_{n=2}^{\infty} \frac{\tau^n}{n!} (j(\vec{\omega}))^{n-2} \right) \vec{\beta}, \end{aligned}$$

with the usual convention that $(j(\vec{\omega}))^0$ is the unit matrix.

The physical meaning of this one-parameter subgroup of the Galilean group can be understood as follows. Let us call *fixed* the affine Euclidean reference frame of space $(O, \vec{e}_x, \vec{e}_y, \vec{e}_z)$ used to represent, at time $t = 0$, a point in space by a vector \vec{r} or by its three components x , y and z . Let us set $\tau = \frac{t}{\varepsilon}$. For each time $t \in \mathbb{R}$, the action of $A(\tau) = A\left(\frac{t}{\varepsilon}\right)$ maps the fixed reference frame $(O, \vec{e}_x, \vec{e}_y, \vec{e}_z)$ onto another affine Euclidean reference frame $(O(t), \vec{e}_x(t), \vec{e}_y(t), \vec{e}_z(t))$, which we call the *moving* reference frame. The velocity and the acceleration of the relative motion of the moving reference

frame with respect to the fixed reference frame is given, at time $t = 0$, by the fundamental vector field associated to the element b of the Lie algebra \mathfrak{G} of the Galilean group: we see that each point in space has a motion composed of a rotation around the axis through O parallel to $\vec{\omega}$, at an angular velocity $\frac{\|\vec{\omega}\|}{\varepsilon}$, and simultaneously a uniformly accelerated motion of translation at an initial velocity $\frac{\vec{\delta}}{\varepsilon}$ and acceleration $\frac{\vec{\beta}}{\varepsilon}$. At time t , the velocity and acceleration of the moving reference frame with respect to its instantaneous position at that time can be described in a similar manner, but instead of O , $\vec{\omega}$, $\vec{\beta}$ and $\vec{\delta}$ we must use the corresponding transformed elements by the action of $A(\tau) = A\left(\frac{t}{\varepsilon}\right)$.

7.3.4 A gas contained in a moving vessel

We consider a mechanical system made by a gas of N point particles, indexed by $i \in \{1, 2, \dots, N\}$, contained in a vessel with rigid, undeformable walls, whose motion in space is given by the action of the one-parameter subgroup G_1 of the Galilean group made by the $A\left(\frac{t}{\varepsilon}\right)$, with $t \in \mathbb{R}$, above described. We denote by m_i , $\vec{r}_i(t)$ and $\vec{v}_i(t)$ the mass, position vector and velocity vector, respectively, of the i -th particle at time t . Since the motion of the vessel containing the gas is precisely given by the action of G_1 , the boundary conditions imposed to the system are invariant by that action, which leaves invariant the evolution space of the mechanical system, is Hamiltonian and projects onto a Hamiltonian action of G_1 on the symplectic manifold of motions of the system. We can therefore consider the generalized Gibbs states of the system, as discussed in 7.1. We must evaluate the momentum map J of that action and its coupling with the element $b \in \mathfrak{G}$. As in 6.3.1 we will neglect, for that evaluation, the contributions of the collisions of the particles between themselves and with the walls of the vessel. The momentum map can therefore be evaluated as if all particles were free, and its coupling $\langle J, b \rangle$ with b is the sum $\sum_{i=1}^N \langle J_i, b \rangle$ of the momentum map J_i of the i -th particle, considered as free, with b . We have

$$\langle J_i(\vec{r}_i, t, \vec{v}_i, m_i), b \rangle = m_i \left(\vec{\omega} \cdot (\vec{r}_i \times \vec{v}_i) - (\vec{r}_i - t \vec{v}_i) \cdot \vec{\beta} + \vec{v}_i \cdot \vec{\delta} - \frac{1}{2} \|\vec{v}_i\|^2 \varepsilon \right).$$

Following Souriau [55], chapter IV, pages 299–303, we observe that $\langle J_i, b \rangle$ is invariant by the action of G_1 . We can therefore define \vec{r}_{i0} , t_0 and \vec{v}_{i0} by setting

$$\begin{pmatrix} \vec{r}_{i0} & \vec{v}_{i0} \\ t_0 & 1 \\ 1 & 0 \end{pmatrix} = \exp\left(-\frac{t}{\varepsilon} b\right) \begin{pmatrix} \vec{r}_i & \vec{v}_i \\ t & 1 \\ 1 & 0 \end{pmatrix}$$

and write

$$\langle J_i(\vec{r}_i, t, \vec{v}_i, m_i), b \rangle = \langle J_i(\vec{r}_{i0}, t_0, \vec{v}_{i0}, m_i), b \rangle.$$

The vectors \vec{r}_{i0} and \vec{v}_{i0} have a clear physical meaning: they are the vectors \vec{r}_i and \vec{v}_i as seen by an observer moving with the moving affine Euclidean reference frame $(O(t), \vec{e}_x(t), \vec{e}_y(t), \vec{e}_z(t))$. Moreover, as can be easily verified, $t_0 = 0$ of course. We therefore have

$$\begin{aligned} \langle J_i(\vec{r}_i, t, \vec{v}_i, m_i), b \rangle &= m_i \left(\vec{\omega} \cdot (\vec{r}_{i0} \times \vec{v}_{i0}) - \vec{r}_{i0} \cdot \vec{\beta} + \vec{v}_{i0} \cdot \vec{\delta} - \frac{1}{2} \|\vec{v}_{i0}\|^2 \varepsilon \right) \\ &= m_i \left(\vec{v}_{i0} \cdot (\vec{\omega} \times \vec{r}_{i0} + \vec{\delta}) - \vec{r}_{i0} \cdot \vec{\beta} - \frac{1}{2} \|\vec{v}_{i0}\|^2 \varepsilon \right) \end{aligned}$$

where we have used the well known property of the mixed product

$$\vec{\omega} \cdot (\vec{r}_{i0} \times \vec{v}_{i0}) = \vec{v}_{i0} \cdot (\vec{\omega} \times \vec{r}_{i0}).$$

Let us set

$$\vec{U}^* = \frac{1}{\varepsilon} (\vec{\omega} \times \vec{r}_{i0} + \vec{\delta}).$$

Using $\vec{v}_{i0} - \vec{U}^*$ and \vec{U}^* instead of \vec{v}_{i0} , we can write

$$\langle J_i(\vec{r}_i, t, \vec{v}_i, m_i), b \rangle = m_i \varepsilon \left(-\frac{1}{2} \|\vec{v}_{i0} - \vec{U}^*\|^2 - \vec{r}_{i0} \cdot \frac{\vec{\beta}}{\varepsilon} + \frac{1}{2} \|\vec{U}^*\|^2 \right).$$

We observe that the vector \vec{U}^* only depends on ε , $\vec{\omega}$, $\vec{\delta}$, which are constants once the element $b \in \mathcal{G}$ is chosen, and of \vec{r}_{i0} , not on \vec{v}_{i0} . It has a clear physical meaning: it is the value of the velocity of the moving affine reference frame with respect to the fixed affine reference frame, at point \vec{r}_{i0} seen by an observer linked to the moving reference frame. Therefore the vector $\vec{w}_{i0} = \vec{v}_{i0} - \vec{U}^*$ is the *relative velocity* of the i -th particle with respect to the moving affine reference frame, seen by an observer linked to the moving reference frame.

The three components of \vec{r}_{i0} and the three components of $\vec{p}_{i0} = m_i \vec{w}_{i0}$ make a system of Darboux coordinates on the six-dimensional symplectic manifold (M_i, ω_i) of motions of the i -th particle. With a slight abuse of notations, we can consider the momentum map J_i as defined on the space of motions of the i -th particle, instead of being defined on the evolution space of this particle, and write

$$\langle J_i(\vec{r}_{i0}, \vec{p}_{i0}), b \rangle = -\varepsilon \left(\frac{1}{2m_i} \|\vec{p}_{i0}\|^2 + m_i f_i(\vec{r}_{i0}) \right), \quad \vec{p}_{i0} = m_i \vec{w}_{i0} = m_i (\vec{v}_{i0} - \vec{U}^*), \quad (*)$$

and

$$f_i(\vec{r}_{i0}) = \vec{r}_{i0} \cdot \frac{\vec{\beta}}{\varepsilon} - \frac{1}{2\varepsilon^2} \|\vec{\omega} \times \vec{r}_{i0}\|^2 - \frac{\vec{\delta}}{\varepsilon} \cdot \left(\frac{\vec{\omega}}{\varepsilon} \times \vec{r}_{i0} \right) - \frac{1}{2\varepsilon^2} \|\vec{\delta}\|^2.$$

The above equality (*) is well suited for the determination of generalized Gibbs states of the system. Let $k \in \mathbb{R}$ be a real. For each $i \in \{1, \dots, N\}$, the integral on the manifold of motions of the i -th particle, with respect to the Liouville measure λ_{ω_i} , of the function $\exp(-\langle J_i, kb \rangle)$, depending on kb as a parameter, is normally convergent in the sense of 7.1.2 if and only if $k\varepsilon < 0$. It means that the set of generalized temperatures, for the action of the one-dimensional group G_1 on the manifold of motions of the i -th particle, is the half-line

$$\Omega = \{kb \mid k \in \mathbb{R} \text{ such that } k\varepsilon < 0\},$$

contained in the Lie algebra \mathcal{G}_1 of G_1 . By replacing eventually b by its opposite, which does not change the one-dimensional group G_1 , we can arrange things in such a way that $\varepsilon < 0$. The matrix b itself is then a generalized temperature, for which we can calculate the partition function and all the generalized thermodynamic functions of the gas made by the i -th particle, for all $i \in \{1, \dots, N\}$. We have

$$P_i(b) = \int_{M_i} \exp(-\langle J_i, b \rangle) d\lambda_{\omega_i}, \quad E_{J_i}(b) = \frac{1}{P_i(b)} \int_{M_i} J_i \exp(-\langle J_i, b \rangle) d\lambda_{\omega_i}.$$

The generalized Gibbs state determined by b (7.1.2) has the smooth density, with respect to the Liouville measure $\prod_{i=1}^N \lambda_{\omega_i}$ on the symplectic manifold of motions $\Pi_{i=1}^N (M_i, \omega_i)$,

$$\rho(b) = \prod_{i=1}^N \rho_i(b), \quad \text{with } \rho_i(b) = \frac{1}{P_i(b)} \exp(-\langle J_i, b \rangle).$$

The partition function, whose expression is

$$P(b) = \prod_{i=1}^N P_i(b),$$

can be used, with the help of the formulae given in 7.2, to determine all the generalized thermodynamic functions of the gas in a generalized Gibbs state.

7.3.5 Remarks.

1. The physical meaning of the parameter ε which appears in the expression of the matrix b is clearly apparent in the above expression (*) of $\langle J_i, b \rangle$:

$$\varepsilon = -\frac{1}{kT},$$

T being the absolute temperature and k the Boltzmann's constant.

2. The same expression (*) above shows that the relative motion of the gas with respect to the moving vessel in which it is contained, seen by an observer linked to that moving vessel, is described by a Hamiltonian system in which the kinetic and potential energies of the i -th particle are, respectively, $\frac{1}{2m_i} \|\vec{p}_{i0}\|^2$ and $m_i f_i(\vec{r}_{i0})$. This result can be obtained in another way: by deriving the Hamiltonian which governs the relative motion of a mechanical system with respect to a moving frame, as used by Jacobi [20] to determine the famous Jacobi integral of the restricted circular three-body problem (in which two big planets move on concentric circular orbits around their common center of mass, and a third planet of negligible mass moves in the gravitational field created by the two big planets).

3. The generalized Gibbs state of the system imposes to the various parts of the system, *i.e.*, to the various particles, to be at the same temperature $T = -\frac{1}{k\varepsilon}$ and to be statistically at rest in the same moving reference frame.

7.3.6 Three examples

1. Let us set $\vec{\omega} = 0$ and $\vec{\beta} = 0$. The motion of the moving vessel containing the gas (with respect to the so called *fixed reference frame*) is a translation at a constant velocity $\frac{\vec{\delta}}{\varepsilon}$. The function $f_i(\vec{r}_{i0})$ is then a constant. In the moving reference frame, which is an inertial frame, we recover the thermodynamic equilibrium state of a monoatomic gas discussed in 6.3.1.

2. Let us set now $\vec{\omega} = 0$ and $\vec{\delta} = 0$. The motion of the moving vessel containing the gas (with respect to the so called *fixed reference frame*) is now an uniformly accelerated translation, with acceleration $\frac{\vec{\beta}}{\varepsilon}$. The function $f_i(\vec{r}_{i0})$ now is

$$f_i(\vec{r}_{i0}) = \vec{r}_{i0} \cdot \frac{\vec{\beta}}{\varepsilon}.$$

In the moving reference frame, which is no more inertial, we recover the thermodynamic equilibrium state of a monoatomic gas in a gravity field $\vec{g} = -\frac{\vec{\beta}}{\varepsilon}$ discussed in 6.3.2.

3. Let us now set $\vec{\omega} = \omega \vec{e}_z$, $\vec{\beta} = 0$ and $\vec{\delta} = 0$. The motion of the moving vessel containing the gas (with respect to the so called *fixed reference frame*) is now a rotation around the coordinate z axis at a constant angular velocity $\frac{\omega}{\varepsilon}$. The function $f_i(\vec{r}_{i0})$ is now

$$f_i(\vec{r}_{i0}) = -\frac{\omega^2}{2\varepsilon^2} \|\vec{e}_z \times \vec{r}_{i0}\|^2.$$

The length $\Delta = \|\vec{e}_z \times \vec{r}_{i0}\|$ is the distance between the i -th particle and the axis of rotation of the moving frame (the coordinate z axis). Moreover, we have seen that $\varepsilon = \frac{-1}{kT}$. Therefore in the generalized Gibbs state, the probability density $\rho_i(b)$ of presence of the i -th particle in its symplectic manifold of motion M_i, ω_i , with respect to the Liouville measure λ_{ω_i} , is

$$\rho_i(b) = \frac{1}{P_i(b)} \exp(-\langle J_i, b \rangle) = \text{Constant} \cdot \exp\left(-\frac{1}{2m_i kT} \|\vec{p}_{i0}\|^2 + \frac{m_i}{2kT} \left(\frac{\omega}{\varepsilon}\right)^2 \Delta^2\right).$$

This formula describes the behaviour of a gas made of point particles of various masses in a centrifuge rotating at a constant angular velocity $\frac{\omega}{\varepsilon}$: the heavier particles concentrate farther from the rotation axis than the lighter ones.

7.3.7 Other applications of generalized Gibbs states

Applications of generalized Gibbs states in Thermodynamics of Continua, with the use of affine tensors, are presented in the papers by G. de Saxcé [49, 50].

Several applications of generalized Gibbs states of subgroups of the Poincaré group were considered by J.-M. Souriau. For example, he presents in his book [55], chapter IV, page 308, a generalized Gibbs state which describes the behaviour of a gas in a relativistic centrifuge, and in his papers [56, 57], very nice applications of such generalized Gibbs states in Cosmology.

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