

Geometry of Phase Space Structures and its Properties

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(Received December 16, 2024, Accepted February 18, 2025)

Abstract: In this paper, we have discussed Geometry of phase space structures and its properties to be expected Conjugate moment; Statistical ensembles in phase space; Phase integral; Motivation for Specific Phase Space Structures; Thermodynamics and statistical mechanics. The Manifold-Based model decline techniques discussed are theoretically based lying on Slow Invariant Manifolds. It engrosses ordinary differential equations and in general dynamical systems during accumulation to Separatrices; Semi-quantum Riemannian geometry; Quantisation of the metric and Levi-Civita connection.

Keywords: Geometry, Phase Space, Manifolds and Dynamical systems.
2020 AMS Subject Classification: 53B15, 53C55.

1. Introduction

The notion of phase space was developed in the late 19th century by Ludwig Boltzmann, Henri Poincaré, and Josiah Willard Gibbs. In dynamical system theory (Mathematical modeling), a phase space is a space in which all likely states of a system are represented, with each likely state equivalent to one unique point in the phase space. For mechanical systems (Physics), the phase space regularly consists of all likely values of position and momentum variables. In a phase space, every degree of freedom or parameter of the system is represented as an axis of a multidimensional space; a one-dimensional system is called a phase line, while a two-dimensional system is called a phase plane. For every possible state of the system or allowed combination of values of the system's parameters, a point is included in the multidimensional space. The system's evolving state over time traces a path (a phase space trajectory for the system) through the high-dimensional space.

In mathematical modeling, we translate problems arising, e.g., in engineering, biology, physics, and chemistry into the mathematical language.

This serves not only to represent reality but also to make predictions, find answers, optimize processes, and to provide us with useful insights. With the rise of computers in the 20th century, the evaluation of such models became more convenient and faster¹⁻³.

Also, scientific issues and progress led to more accurate but more complicated mathematical models. Despite ever increasing processing power of modern computers, the complexity of realistic models often prevents the best computers from detailed computations in decent time. One of such rather complicated models emerges in the optimal control of chemical reaction mechanisms. Chemical kinetics is typically modeled by Ordinary Differential Equations (ODEs). In optimal control, these differential equations are parameterized by some control variables¹⁻³.

2. Geometry of Phase Space Structures and its properties

Conjugate moment: In classical mechanics, any choice of generalized coordinate's q_i for the position (i.e. coordinates on configuration space) defines conjugate generalized moment a p_i which together defines coordinates on phase space. More abstractly, in classical mechanics phase space is the cotangent bundle of configuration space, and in this interpretation the procedure above expresses that a choice of local coordinates on configuration space induces a choice of natural local Darboux coordinates for the standard symplectic structure on a cotangent space.

Statistical ensembles in phase space: The motion of an ensemble of systems in this space is studied by classical statistical mechanics. The local density of points in such systems obeys Liouville's theorem, and so can be taken as constant. Within the context of a model system in classical mechanics, the phase space coordinates of the system at any given time are composed of all of the system's dynamic variables. Because of this, it is possible to calculate the state of the system at any given time in the future or the past, through integration of Hamilton's or Lagrange's equations of motion.

Phase plot: A plot of position and momentum variables as a function of time is sometimes called a phase plot or a phase diagram. However the latter expression, "phase diagram", is more usually reserved in the physical sciences for a diagram showing the various regions of stability of the thermodynamic phases of a chemical system, which consists of pressure, temperature, and composition.

Phase integral: In classical statistical mechanics (continuous energies) the concept of phase space provides a classical analog to the partition function (sum over states) known as the phase integral. Instead of summing the

Boltzmann factor over discretely spaced energy states (defined by appropriate integer quantum numbers for each degree of freedom) one may integrate over continuous phase space. Such integration essentially consists of two parts: integration of the momentum component of all degrees of freedom (momentum space) and integration of the position component of all degrees of freedom (configuration space). Once the phase integral is known, it may be related to the classical partition function by multiplication of a normalization constant representing the number of quantum energy states per unit phase space. This normalization constant is simply the inverse of Planck's constant raised to a power equal to the number of degrees of freedom for the system.

Motivation for Specific Phase Space Structures: Envision a map where all sources of water, creeks, rivers, and seas are charted. It is observed that many sources of water bundle into a creek. Creeks bundle into rivers and rivers into seas. For the long-term behavior of the water dynamics from dropping down on a mountain through to a sea or ocean, it is intuitive to follow the closest river on the map and neglect the exact path of a simple water drop through a creek to the river. Waterfalls very quickly from the top of a mountain to a valley where it bundles into a river. Once in a river, the cruising speed is much slower than before and remains slow on the way to the sea. Explained into mathematical terms, this directs to the idea of model reduction, bundling behavior, and multiple time scales. For the long-term behavior of a water drop, it is sufficient to know which river it enters. This is the basic idea of model reduction.

Thermodynamics and statistical mechanics: In thermodynamics and statistical mechanics contexts, the term phase space has two meanings: for one, it is used in the same sense as in classical mechanics. If a thermodynamic system consists of N particles, then a point in the $6N$ -dimensional phase space describes the dynamic state of every particle in that system, as each particle is associated with three-position variables and three momentum variables.

The phase space can also submit to the space that is parameterized by the macroscopic states of the system, such as pressure, temperature, etc. For instance, one may view the pressure-volume diagram or entropy-temperature diagrams as describing part of this phase space. A point in this phase space is correspondingly called a macro state.

3. Dynamical Systems

The Manifold-Based model decline techniques discussed are theoretically based lying on Slow Invariant Manifolds². It engrosses ordinary differential

equations and in general dynamical systems. We provide a basic concept of dynamical systems by the following definition. Basically, it is a mapping that describes the evolution of a certain state x with time t .

Definition 3.1: Let $(M; d)$ be a metric space. A dynamical system (or flow) ϕ is a mapping $\phi: \mathbb{R} \times M \rightarrow M, (t, x) \rightarrow \phi(t, x)$ such that

(D1) $\phi(0, x) = x \forall x \in M$,

(D2) $\phi(t + s, x) = \phi(t, \phi(s, x)) \forall t, s \in \mathbb{R}, x \in M$,

(D3) ϕ is a continuous mapping.

4. Slow Invariant Manifolds

In multi-scale systems, a part of the dynamics evolves much faster than the rest of the dynamics². For instance, in chemical reactions, some partial reactions have a time scale in the range of nanoseconds while other reactions occur in multiple seconds. If dynamics are modeled by differential equations, this timescale separation leads to so-called stiff differential equations. Explicit numerical methods typically are unstable for such problems. Even modern computers and the usage of sophisticated numerical tools cannot overcome the challenges of numerical stiffness and high-dimensionality.

Mathematically, this is modeled by optimal control problems. Central object of optimal control problems are differential equations that can be controlled by some control variables. In optimal control problems, a desired cost function depending on the controls and states is minimized. The problem is constrained by differential equations. Thus, optimal control problems inherit the difficulties of handling differential equations. To this end, it seems natural to investigate whether numerical manifold-based model reduction techniques can be applied to optimal control problems as well.

5. Separatrices

The concentrations of chemical species are represented by real numbers⁴. Therefore, if reaction mechanisms are modeled by ODEs, all considered variables were real-valued as well. A look at complex valued dynamical systems reveals that other phase space structures than SIMs are important and significant for long-term and asymptotic behavior. So far, we only considered dissipative dynamical systems like chemical reactions, i.e., in which the entropy does not decrease and SIMs as phase space structures. Riemann showed that the Riemann functions:

$$X(z) = \sum_{n=1}^{\infty} \frac{1}{n^z}, \quad z = C.$$

plays an essential role in analytical number theory since the location of its zeros allows locating the prime numbers within the natural numbers. One of the millennium problems is the Riemann hypothesis, which asserts that all non-trivial zeros of the Riemann function are on the critical line $z = 1/2$.

6. Semi-quantum Riemannian geometry

We will work in a local coordinate basis for our manifold M so that⁵

$$\{a, b\} = \omega^{ij} a_{,i} b_{,j} , \quad \nabla_j dx^i = - \Gamma_{jk}^i dx^k$$

Where Γ are the Christoffel symbols of our (partial) linear connection ∇ . Then from the identity given by⁷ as

$$(6.1) \quad d\{a, b\} = \nabla_{\hat{a}} db - \nabla_{\hat{b}} da \quad \text{and} \quad \omega^{ij}_{;m} + \omega^{ik} T_{km}^j - \omega^{jk} T_{km}^i = 0,$$

where $T_{jk}^i = \Gamma_{jk}^i - \Gamma_{kj}^i$ is the torsion tensor of ∇ and $(;)$ is with respect to ∇ . Given this identity, the requirement that the antisymmetric bivector ω^{ij} defines a Poisson Tensor becomes⁷ as

$$(6.2) \quad \sum_{cyclic (i,j,k)} \omega^{im} \omega^{jn} T_{mn}^k = 0.$$

Again depending only on the torsion. We will verbalize throughout about a Poisson Tensor ω and ∇ Poisson-compatible.

7. Quantisation of the metric and Levi-Civita connection

Here we suppose that (M, ω, ∇) above has additional structure $(g, \hat{\nabla})$ where g is a Riemannian (or pseudo-Riemannian) metric and $\hat{\nabla}$ is the Levi-Civita connection. The condition in ⁷ for the construction of a quantum metric comes out as the very reasonable requirement

$$(7.1) \quad \nabla g = 0.$$

That our Poisson connection is compatible with g . It corresponds at the quantum level to the quantum metric being central and we assume the condition from now on. We build the quantum metric in two stages. First, the functorial choice is

$$(7.2) \quad gQ = q^{-1} \Omega^1, \quad \Omega^1(g) = g_{ij} dx^i \otimes_1 dx^j + \frac{\lambda}{2} \omega^{ij} g_{pm} \Gamma_{iq}^p \Gamma_{jn}^q dx^m \otimes_1 dx^n.$$

One has $Q g Q = 0$, so this is quantum metric compatible. We want our quantum metric to be quantum symmetric in the sense of killed by the quantum wedge product but we find

$$(7.3) \quad \wedge_1 gQ = \lambda R ; R = H^{ij} g_{ij},$$

where explicitly

$$(7.4) \quad R = \frac{1}{2} R_{mn} dx^n \wedge dr^m, R_{mn} = \frac{1}{2} g_{ij} w^{is} (T_{nm;s}^j - R_{nms}^j - R_{mns}^j).$$

One can therefore either live with this or, which we do, define

$$(7.5) \quad g_1 = g_Q - \frac{\lambda}{4} g_{ij} w^{is} (T_{nm;s}^j - R_{nms}^j - R_{mns}^j) dx^m \otimes_1 dx^n.$$

As the quantum metric, this now has $\Lambda_1(g_1) = 0$.

Finally, write the classical Levi-Civita connection as $\hat{\nabla} = \nabla + S$, where

$$(7.6) \quad S_{jk}^i = \frac{1}{2} g^{im} (T_{mjk} - T_{jkm} - T_{kjm}).$$

Is the contorsion tensor built from the torsion $\mathbf{T}$ of ∇ . We do not want to give all the details but the main idea in [Beggs and Majid (2014)] is to functorially quantise the contorsion to a quantum one $Q(S)$ and also to allow a further $O(\lambda)$ adjustment by a classical tensor K , i.e. we search for the quantum-Levi Civita connection in the form

$$(7.7) \quad \nabla_1 = \nabla Q + Q(S) + \lambda K.$$

Theorem 7.1: *There is a unique quantum connection ∇_1 which is quantum torsion free and for which the symmetric part in the last two factors of $\nabla_1 g_1$ vanishes.*

Proof: We have $\nabla_1 g_1 = 0$ entirely if and only if ⁷

$$\hat{\nabla} \mathcal{R} + \omega^{ij} g_{rs} S_{jn}^s (R_{mki}^r + S_{km;i}^r) dx^k \otimes dx^m \wedge dx^n = 0.$$

The theorem says that there is always a unique best-possible quantum Levi-Civita Connection but in general there could be an antisymmetric correction in the sense

$$(id \otimes \wedge) \nabla_1 g_1 = O(\lambda).$$

As a new feature of quantum geometry. The condition for this correction to vanish is the one stated in the theorem but there are examples such as the ax symmetrically quantized Schwarzschild black hole in [Beggs and Majid (2014)], where we show that the correction cannot vanish for a large class of Poisson-connections ∇ .

We will be interested only in the canonical special case $S = T = 0$ of the above, where the $\nabla = \hat{\nabla}$. In this case

$$\mathcal{R} = -\frac{1}{2} g_{ij} \omega^{is} R_{nms}^j dx^m \wedge dx^n.$$

And the best possible quantum Levi-Civita connection is just ∇_Q itself. The condition in the Theorem above is that this is covariantly constant. This holds for example for any Kaehler-Einstein manifold.

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