Non-commutative Geometry and Kinetic Theory of Open Systems

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Abstract

The basic mathematical assumptions for autonomous linear kinetic equations for a classical system are formulated, leading to the conclusion that if they are differential equations on its phase space M, they are at most of the 2nd order. For open systems interacting with a bath at canonical equilibrium they have a particular form of an equation of a generalized Fokker-Planck type. We show that it is possible to obtain them as Liouville equations of Hamiltonian dynamics on M with a particular non-commutative differential structure, provided certain geometric in character, conditions are fulfilled. To this end, symplectic geometry on M is developped in this context, and an outline of the required tensor analysis and differential geometry is given. Certain questions for the possible mathematical interpretation of this structure are also discussed.

1 Introduction

The understanding and description of irreversible evolution of macroscopic systems, presumably towards equilibrium states is the aim of kinetic theory. This is done by formulating appropriate kinetic equations giving the time evolution of the state of the system which loosely speaking, is assumed to be some probability measure on the space of variables describing the system, which henceforth will be called its phase-space. Observables are assumed to be well-behaved phase-space functions and experimental results refer to expectation values obtained via a bilinear (or sesquilinear) form on the cartesian product of the spaces of states and observables. Thus at the very heart of kinetic theory a probabilistic view point is rooted, the precise interpretation of which is often a matter of debate.

Theoretically speaking, kinetic equations are derived by following two different procedures:

(i) stochastic arguments, based on some presumably plausible assumptions on the behaviour of a large number of microscopic events characterising the system.

(ii) application of more or less systematic approximation schemes on the exact microscopic dynamics of the system under consideration.

Typical examples for (i) are the Fokker-Planck and Kramers equations (e.g. [1] ch.VIII). The first refers to the probability distribution function (p.d.f.) of the velocity of a heavy Brownian particle suspended in an equilibrium medium of light particles, the second one, to the p.d.f. of its phase-space position under the presence of an external field. The basic assumptions for their derivation are that the microscopic dynamics of the Brownian particle are governed by Langevin's equation and that its p.d.f. is a Markovian diffusion process (see e.g. [2] ch.II, [3]). This procedure usually leads to *model* equations that are easier to study than the *assumed* more fundamental equations following from exact dynamics by (ii). Mathematically speaking, this procedure essentially *replaces exact dynamics by stochastic differential equations* which in turn imply evolution equations for the p.d.f. of the system (e.g. [4] ch.4, [5] ch.9). Though interesting and important from both the mathematical and physical point of view, it seems that one has to know somehow the kinetic equation he wants to derive and modify accordingly the corresponding dynamics. Moreover the modification is not easily interpreted physically (see the discussion following (3.1) below). That is, it seems that there is no general prescription of how this modification has to be carried out. In this paper, starting from mathematically totally different concepts we do arrive at results that may be interpreted stochastically, at the same time giving hints on the nature of such a general prescription (cf. the discussion following (3.1) below).

Typical examples for (ii) are the Boltzmann equation for dilute classical gases (or its quantum weak-coupling analogue, Pauli's equation) or the Landau and Balescu-Lenard equations for neutral plasmas, as they are derived from Liouville's (or von Neumann's) equations by using either iteration schemes and projection operator methods, or by using its equivalent, the BBGKY hierarchy of equations truncated on the basis of physical considerations.[1]

Although many specific equations can be derived by mathematically satisfactory (or even rigorous) methods in some particular limit of appropriate parameters of the system (for a survey see [33]), it is true that *any approximation scheme, leading to satisfactory kinetic equations for particular classes of systems, runs into trouble as long as one tries to extend it to other systems and/or higher order of approximation* ([12], [13] §5). For

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[1]See e.g. [6] §§30, 41, [7] ch.20, [8] ch.IX, [9] §2.4, [10] §§4.3, 4.6, [11] §VI.

instance the linearized Landau equation follows for spatially homogeneous plasmas as a 2nd order approximation in the plasma parameter to the Liouville equation (plus some additional assumptions which need not be discussed here). Any effort to find its generalization either in higher order of approximation and/or for inhomogeneous systems, runs into difficulties (e.g. equations violating the positivity of p.d.f or having no H-theorem, are obtained — see e.g. [14] in connection with [13] §5), or involves highly ad hoc steps which are sometimes hidden in the calculations (see e.g. [15] in connection with §2 below).

Although one may be tempted to accept that there is no reason to expect that equations in an approximate theory share all properties of the corresponding equations in the exact theory, in kinetic theory things are more complicated since the exact theory in this case is simply (classical or quantum) dynamics; however as it stands, microscopic dynamics of a system with a very large number of degrees of freedom is useless as a macroscopic theory since it does not incorporate irreversible evolution and its relation to a theory dealing with macroscopically defined quantities is remote, or at least not straightforward. Moreover from what has been said above, the situation is even worse, since it often happens that equations obtained at a lower level of approximation (e.g. with respect to expansion in some parameter) exhibit the correct properties, which however disappear in any higher level of approximation![2]

In our opinion this is an inevitable consequence of the philosophy underlying kinetic theory, namely that *irreversible evolution* is simply an approximation to the exact (classical or quantum) *reversible dynamics*. To put it differently, the *aim* of kinetic theory (description of macroscopic irreversible evolution) seems not to be *compatible* with its *assumed fundamental laws* (reversible microscopic dynamics), at least in a straightforward manner. Therefore it seems necessary that a fundamentally different approach to kinetic theory may not be worthless!

2 Mathematical assumptions underlying kinetic theory and their implications.

As already mentioned, at the very root of kinetic theory lies a probabilistic interpretation. Using this as a motivation and in order to clarify the difficulties noticed in the previous paragraph, we here describe the basic assumptions for a kinetic equation to be in principle, acceptable, and conditions under which an explicit general form can be obtained. We restrict the discussion to *linear, autonomous* kinetic equations, which include kinetic equations for the important class of *open systems*. To be more specific, we consider *clas-*

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[2]See e.g. equations following from expansion of Liouville's equation or the so-called generalized master equation [10] §2.3, [12] §2, [13] §5, [27] in connection with the last paragraph of the next section. See also [34] for expansions of the Boltzmann equation.

sical systems, though similar results are known for quantum systems as well ([19], [16] Theorem 4.2).

We assume that

(i) The phase-space M is a locally compact, Hausdorff topological space (e.g. the phase-space of a Hamiltonian system).

(ii) Observables A are in $C(M, \mathbb{C})$ the space of complex-valued continuous functions on M, having a finite limit at infinity.

(iii) States ℓ are positive linear functionals on the observables, their values $\ell(A)$ giving expectations. Since positivity of ℓ, implies its boundedness in the supremum norm (e.g. [21] p.106–107), states belong to $C^*(M, \mathbb{C})$, the Banach dual with respect to this norm, which is the space of (regular) complex Borel measures on M.

(iv) Kinetic equations for the observables have well-posed initial value problem, i.e. uniqueness and continuous dependence of solutions on the initial data hold. Moreover, expectation values are continuous in time. These imply that solutions of a kinetic equation define strongly continuous semigroups of linear operators on the space of observables and that the corresponding adjoint equation defines such a semigroup on the state space.[3]

(v) The adjoint semigroup conserves positivity and normalization of the states, i.e. initial probability measures retain their character for all positive times.

These plausible assumptions imply that the solutions of a kinetic equation for the observables define a Markov semigroup, i.e. a strongly continuous, positivity and normalization preserving one-parameter semigroup of operators on $C(M, \mathbb{C})$ [27]. The terminology stems from the fact that such semigroups are in one to one correspondence with (time-homogeneous) stochastically continuous Markov processes described by a transition probability distribution $p(t, x, E)$, which for each t, x is a regural probability Borel measure on M (see e.g. [23] p.399, [24] Theorem 2.1, for outline of a proof). If we further *assume* that M is an n-dimensional differential manifold, the generator of the semigroup is defined on C^2-functions and that a Lindenberg's type condition holds,

$$\lim_{t \to 0^+} \frac{p(t, x, E)}{t} = \chi_E(x) \qquad \text{uniformly in } x,$$

where χ_E is the characteristic function of E, then it can be proved that the kinetic equation for observables (i.e. essentially the generator of the corresponding semigroup)

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[3]Strictly speaking, strong continuity of the latter holds on a smaller subspace, which however uniquelly defines the adjoint semigroup ([22] Theorem 1.36).

has the form[4]

$$\frac{\partial A}{\partial t} = \alpha^{ij}(x)\partial_i\partial_j A + a^i(x)\partial_i A \ , \tag{2.1}$$

where α^{ij}, a^i are continuous, α^{ij} is a non-negative definite matrix function and the summation convention has been used, as it will be done in the sequel.[5] Actually α^{ij}, a^i are related to the diffusion and drift coefficients associated with the corresponding Markov process, given by the first two moments of p.

In many approaches in kinetic theory which lead to satisfactory kinetic equations of the form (2.1), the following condition holds

$$a^i = b^i + X_H^i \ , \tag{2.2}$$

where X_H^i is a *Hamiltonian* vector field. Moreover for *open* (classical or quantum) systems with Hamiltonian H, in interaction with "baths" in canonical equilibrium, the corresponding Hamiltonian function is an integral of the unperturbed motion of the open system, and therefore has in general the form $-(H + F)$ with

$$\{F, H\} = 0 \ , \tag{2.3}$$

$\{ \, , \}$ being the Poisson bracket, or the operator commutator, and the minus sign gives the correct Hamiltonian equation when the system does not interact with the bath.

Moreover

$$\partial_j \alpha^{ij} - b^i = \beta \alpha^{ij} \partial_j H \ , \tag{2.4}$$

where β is proportional to the inverse temperature of the bath.[6] These conditions will be used in section 4.

Substitution of (2.2)–(2.4) in (2.1) gives

$$\frac{\partial A}{\partial t} = -\{H + F, A\} + \partial_i(\alpha^{ij}\partial_j A) - \beta\alpha^{ij}\partial_j H \partial_i A \ . \tag{2.5}$$

The essential conclusion drawn from the above discussion is (in a somewhat nonrigorous language) that *linear autonomous kinetic equations for classical systems, which are differential equations are necessarily at most of the 2nd order with nonnegative-definite leading coefficient and vanishing zeroth order term (cf. eq.(2.1))*.[7]

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[4]See [25] Theorem 5.3 for outline of a proof, and [26] Theorem XIII.53 for a partial generalization — the Lévy-Khinchine formula.

[5]For detailed proofs and more precise formulation of the various conditions see [27].

[6]See e.g. [13] Proposition 4.1, [28] eq.(2.19), [6] p.190, [18] eqs(III.26) and (III.16) together with (III.19), [32] eq.(5.8).

[7]A corresponding result is also known for quantum systems [19], [17], [18]. The special case of the Kramers-Moyal expansion of the linearized Boltzmann equation has been considered in [34].

Since kinetic equations following from microscopic dynamics (see §1) are often differential equations, the above result, severely restricts their form. In particular all methods based on power expansions of the solution of Liouville's equation with respect to some appropriate parameter, usually lead to unacceptable results since each approximation step increases the order of the differential operator by one.[8] In the rest of this paper, we will present a different point of view, motivated by the discussion in the next section.

3 Non-commutative geometry and stochastic calculus.

The usual approach to kinetic theory (method (ii) in Section 1) follows the scheme

Microscopic (Hamiltonian dynamics)

$+$ $\Longrightarrow$ Kinetic equations

Some systematic approximation scheme

On the other hand, method (i) in Section 1, involves no systematic approximation scheme but a modification of microscopic dynamics which become now stochastic differential equations. In our opinion, the weak point in this case is that there is no general method of how to choose the microscopic stochastic differential equations. That is, it seems necessary that one somehow knows the kinetic equation he wants to derive and then writes down the corresponding stochastic equation. However it is not always clear how to interpret the latter.

For instance it would be desirable to be able to derive by method (i) kinetic equations obtained from microscopic Hamiltonian dynamics. However, the latter in general involve operators with derivatives in the q-coordinates (see e.g. [12], [13], [28], [32]). And it is a standard fact that stochastic differentil equations in phase-space involving Wiener processes $\vec{X}_t$ of the form

$$\left(\begin{array}{c} d\vec{q} \\ d\vec{p} \end{array} \right) = \left(\begin{array}{c} \vec{A}_q(\vec{q},\vec{p})\,dt + \mathbf{F}_q(\vec{q},\vec{p}) \cdot d\vec{X}_t^q \\ \vec{A}_p(\vec{q},\vec{p})\,dt + \mathbf{F}_p(\vec{q},\vec{p}) \cdot d\vec{X}_t^p \end{array} \right) \,, \tag{3.1}$$

imply such derivatives in the corresponding kinetic equation if $\mathbf{F}_q \neq 0$ (see e.g. [4] §4.3.3). However in many cases, one would like to interpret $d\vec{q}/dt$ simply as a velocity, all dynamics being incorporated in $d\vec{p}/dt$ (e.g. the velocity of a Brownian particle), in which case the above stochastic equation (3.1) is not easily interpreted physically.

In the next sections we outline *another approach* in which *the Hamiltonian character of microscopic dynamics is retained, but instead of approximation schemes, we make the*

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[8]See e.g. [10] §2.4 eq.(2.199), [1] p.215, §IX.6 particularly p.280.

fundamental assumption that observables are now defined on a manifold with noncommutative geometrical structure. As it will be explained, this may be interpreted as a stochastic dynamical structure, though it is not known if this is necessary. Nevertheless, the formulation developped in the next section is closely related to what may be called a differential geometric approach to stochastic calculus[9] though this relation will be further explored in another paper.

The *mathematical* motivation for introducing noncommutative geometrical structure, stems from the fact that in the one-dimensional version of (3.1), X_t being a Wiener process (i.e. Langevin's equation) the usual associative product between differential forms spanned by dt, dX_t and functions of t, X_t, implies that stochastic differentiation does not obey Leibniz's rule for the product of two functions, due to the appearance of 2nd derivatives in Itô's formula for the differential of such functions ([29] §2, particularly eq.(2.4)).However it is possible to define a modified *noncommutative* but still associative product between functions and differential forms such that Leibniz's rule holds ([29] section 3). This product induces a noncommutative differential calculus on the ordinary algebra of functions of t, X_t ([30] section 2) via the basic commutation relations between functions and 1-forms

$$[\mathrm{d}t, t] = [\mathrm{d}t, X_t] = 0 \ ,$$
$$[\mathrm{d}X_t, X_t] = 2\gamma\, \mathrm{d}t \ , \tag{3.2}$$

γ being the diffusion constant appearing in the usual Fokker-Planck equation obtained from Langevin's equation ([29] eq.(3.16)). Eq.(3.2) is readily generalized to a multidimensional Wiener process:

$$[\mathrm{d}t, t] = [\mathrm{d}t, X_t^i] = 0 \ ,$$
$$[\mathrm{d}X_t^i, X_t^j] = b^{ij}\, \mathrm{d}t \ , \tag{3.3}$$

where b^{ij} is a symmetric bilinear form on the space of 1-forms.[10] Therefore (3.3) can be rewritten more generally as

$$[\mathrm{d}f, g] = b(\mathrm{d}f, \mathrm{d}g)\, \mathrm{d}t \ , \tag{3.4}$$

for functions f, g of $\vec{X}_t, t$ and a symmetric, bilinear form with components b^{ij} in the "coordinates" X_t^i and such that $\mathrm{d}t$ lies in its kernel, i.e. $b^{tt} = b^{it} = 0$.

In view of the above discussion, we consider in the next section a $(2n+1)$-dimensional manifold $M \times \mathbb{R}$ and a differential calculus on a subalgebra $\mathcal{A}$ of the algebra of complex-valued functions on $M \times \mathbb{R}$ satisfying (3.4), and outline *the formulation of extended Hamiltonian dynamics as symplectic geometry on $M \times \mathbb{R}$*. The basic result is that *Liouville's*

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[9]See e.g. [37], [38] particularly ch.VI, compare also with the approach in [39].

[10]This is implied by the fact that since d satisfies Leibniz's rule, $[\mathrm{d}X_t^i, X_t^j] = [\mathrm{d}X_t^j, X_t^i]$ which in fact shows that this commutator depends only on $\mathrm{d}X_t^i$, $\mathrm{d}X_t^j$ — see [30] §3.

equation for observables turns out to be of the form (2.1) with conditions (2.2), (2.4) having a simple geometrical meaning. Therefore it may be interpreted as a kinetic equation on the space of observables corresponding to a classical open system with phase-space M.

The construction is coordinate-independent, and presupposes the definition of such fundamental concepts as vector fields, linear connections, symplectic structure and antisymmetric wedge product of forms on the differential calculus defined on $\mathcal{A}$ by (3.3), in close analogy with the corresponding concepts of the ordinary differential geometry.[11] The derivation is *formal* in the sense that no systematic study of the representation theory of (3.3) is made. Its already mentioned relation with stochastic calculus is a possibility, but it is not clear if others exist. A preliminary discussion of this problem is given in section 5.

To make the presentation as transparent as possible, detailed calculations will be given in a subsequent paper in which tensor analysis for the corresponding noncommutative differential calculus is developped systematically. In fact this work constitutes only a first step towards a systematic formulation of kinetic theory as Hamiltonian (symplectic) dynamics in phase-space equipped with a noncommutative geometrical structure.

4   Noncommutative symplectic geometry

Let M be a $2n$-dimensional manifold and $\mathcal{A}$ the algebra of smooth functions on $M \times \mathbb{R}$. The coordinate on $\mathbb{R}$ will be denoted by t. Let $\tilde{\Omega}$ be the universal differential envelope of $\mathcal{A}$, i.e. $\tilde{\Omega}$ is a $\mathbb{Z}$-graded algebra $\tilde{\Omega} = \bigoplus_{r \in \mathbb{Z}} \tilde{\Omega}^r$ with $\tilde{\Omega}^r = \{0\}$ for $r < 0$ and $\tilde{\Omega}^0 = \mathcal{A}$. Then there exists a linear mapping $\tilde{d} : \tilde{\Omega} \to \tilde{\Omega}$ of grade 1, which satisfies

(i) $\tilde{d}1 = 0$, where 1 is the constant function with value 1,

(ii) $\tilde{d}$ satisfies the graded Leibniz rule i.e. $\tilde{d}(\psi\psi') = (\tilde{d}\psi)\psi' + (-1)^r\psi(\tilde{d}\psi')$, for $\psi \in \tilde{\Omega}^r$,

(iii) $\tilde{d}^2 = 0$ on all of $\tilde{\Omega}$ and

(iv) $\mathcal{A}$ and $\tilde{d}\mathcal{A}$ generate $\tilde{\Omega}$.

The universal differential envelope $(\tilde{\Omega}, \tilde{d})$ of $\mathcal{A}$ can be realized as follows (see [40]): think of $\phi \in \tilde{\Omega}^r$ as a function on $(M \times \mathbb{R})^{r+1}$, where for $f \in \tilde{\Omega}^0$ and $a \in M \times \mathbb{R}$ $f(a)$ is the value of f as an element of $\mathcal{A}$ on a and for $a_0, \ldots, a_{r+1} \in M \times \mathbb{R}$ and $\phi \in \tilde{\Omega}^r$ we set

$$(\tilde{d}\phi)(a_0, \ldots, a_{r+1}) := \sum_{k=0}^{r+1} (-1)^k \phi(a_0, \ldots, a_{k-1}, a_{k+1}, \ldots, a_{r+1}) \ .$$

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[11]For details on the systematic definition and presentation of general results in noncommutative geometry on a commutative algebra, see [30], particularly §§2,3.

Furthermore for $\phi \in \tilde{\Omega}^r$, $\psi \in \tilde{\Omega}^s$ and $a_0, \dots a_{r+s} \in M \times \mathbb{R}$ we set

$$(\phi\psi)(a_0, \dots, a_{r+s}) := [\phi(a_0, \dots, a_r)][\psi(a_r, \dots, a_{r+s})] \ ,$$

for any non negative integers r, s. According to these rules

$$(f\tilde{d}g\, h)(a, b) = f(a)[g(b) - g(a)]h(b) \ , \tag{4.1}$$

and hence $\tilde{d}f\, g \neq g\tilde{d}f$. On the $\mathcal{A}$-bimodule of 1-forms $\tilde{\Omega}^1$ we define a new product $\tilde{\bullet} : \tilde{\Omega}^1 \times \tilde{\Omega}^1 \to \tilde{\Omega}^1$ as follows: for $\alpha, \beta \in \tilde{\Omega}^1$ and $a, b \in M \times \mathbb{R}$ we set

$$(\alpha\tilde{\bullet}\beta)(a, b) := \alpha(a, b)\, \beta(a, b) \ .$$

Note that

$$(f_1\alpha f_2)\tilde{\bullet}(g_1\beta g_2) = f_1 g_1 (\alpha\tilde{\bullet}\beta) f_2 g_2 \ ,$$

and $[\tilde{d}f, g] = \tilde{d}f\tilde{\bullet}\tilde{d}g$. The universality of $(\tilde{\Omega}, \tilde{d})$ is expressed by the property that, if (Ω, d) is any differential algebra on $\mathcal{A}$, then there is a graded-algebra homomorphism $\pi : \tilde{\Omega} \to \Omega$ of grade 0 such that $\pi|\tilde{\Omega}^0 = \mathrm{id}_\mathcal{A}$ and $d \circ \pi = \pi \circ \tilde{d}$ (cf. [30] §3.1).

Let $\tilde{b} : \tilde{\Omega}^1 \times \tilde{\Omega}^1 \to \mathcal{A}$ be a symmetric left-right $\mathcal{A}$-bilinear form i.e. $\tilde{b}(f_1\alpha f_2, g_1\beta g_2) = f_1 g_1\, \tilde{b}(\alpha, \beta)\, f_2 g_2$ and assume that $\tilde{d}t$ lies in the kernel of $\tilde{b}$. Let also $\mathcal{I}$ denote the differential ideal of $\tilde{\Omega}$ generated by $\alpha\tilde{\bullet}\beta - \tilde{d}t\, \tilde{b}(\alpha, \beta)$, then we set $\Omega := \tilde{\Omega}/\mathcal{I}$ and $\pi : \tilde{\Omega} \to \Omega$ for the canonical projection. Since $\mathcal{I}$ is differential the operator $d : \Omega \to \Omega$ given by $d = \pi \circ \tilde{d}$ is well defined, and because $\tilde{d}t$ lies in the kernel of $\tilde{b}$, a symmetric left-right $\mathcal{A}$-bilinear form $b : \Omega \times \Omega \to \mathcal{A}$ is uniquelly defined by $b \circ (\pi \times \pi) = \tilde{b}$.

Now set

$$df \bullet dg := [df, g] \ , \tag{4.2}$$

and extend by left-right $\mathcal{A}$-bilinearity, then it is easy to see that $\pi(\tilde{\alpha}\tilde{\bullet}\tilde{\beta}) = \alpha \bullet \beta$, where $\alpha = \pi(\tilde{\alpha})$ and similarly for β. Obviously we have

$$\alpha \bullet \beta = dt\, b(\alpha, \beta) \ . \tag{4.3}$$

This is but a special case of the general procedure used to relate $(\tilde{\Omega}, \tilde{d})$ to any other differential calculus (Ω, d) via an $\mathcal{A}$-bimodule homomorphism π, with $\mathcal{I} = \ker \pi$ and induce $\bullet$ on Ω^1 by $\tilde{\bullet}$ on $\tilde{\Omega}^1$ (cf. [30] §3.2). Let ξ^i, $i = 1, \dots, 2n$ be local coordinates on M then the elements of $\mathcal{A}$ can be written locally as functions of t, ξ^i, $i = 1, \dots, 2n$ (see also section 5). If we set $b^{ij} := b(d\xi^i, d\xi^j)$ we find the commutation relations — note that $b(dt, d\xi^i) = b(d\xi^i, dt) = 0$ —

$$[d\xi^i, \xi^j] \ = \ dt b^{ij} \ , \tag{4.4}$$
$$[dt, t] = [dt, \xi^i] = [d\xi^i, t] \ = \ 0 \ . \tag{4.5}$$

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These are special cases of

$$[\mathrm{d}f, g] = \mathrm{d}t \, b(\mathrm{d}f, \mathrm{d}g) \ . \tag{4.6}$$

By (4.2), (4.5) we get for any $f, g, h \in \mathcal{A}$ that

$$\mathrm{d}f \bullet \mathrm{d}g \bullet \mathrm{d}h = 0 \ . \tag{4.7}$$

Applying d on a product of two functions and using (4.6) we obtain

$$\mathrm{d}(fg) = (\mathrm{d}f)g + (\mathrm{d}g)f - \mathrm{d}t \, b(\mathrm{d}f, \mathrm{d}g) \ . \tag{4.8}$$

Considering Ω^1 as a right $\mathcal{A}$ module the dual module $\mathcal{X}$ is a left $\mathcal{A}$ module. We write $\langle X, \alpha \rangle$ for the duality contraction. If we define

$$Xf := \langle X, \mathrm{d}f \rangle \ , \tag{4.9}$$

then we obtain from (4.8)

$$X(fg) = g(Xf) + f(Xg) - b(\mathrm{d}f, \mathrm{d}g)(Xt) \ . \tag{4.10}$$

The elements of $\mathcal{X}$ will be called *vector fields*. It can be proved that as a left $\mathcal{A}$ module $\mathcal{X}$ is free with basis given by $\hat{\partial}_t, \partial_1, \ldots, \partial_{2n}$, where

$$\begin{aligned}
\partial_i &:= \frac{\partial}{\partial \xi^i} \ , \\
\hat{\partial}_t &:= \partial_t - \tfrac{1}{2} b^{ij} \partial_i \partial_j \ .
\end{aligned} \tag{4.11}$$

Thus for $X \in \mathcal{X}$ we have

$$X = \hat{X}^t \, \hat{\partial}_t + X^i \, \partial_i \ , \tag{4.12}$$

with $X^i := (X\xi^i)$, $\hat{X}^t := (Xt)$. More generally it can be proved that for any differential calculus on a differential manifold, satisfying (4.7) vector fields, i.e. elements of $\mathcal{X}$, are second order differential operators without constant term, like (4.12). Thus the name 2nd order calculus is justified in this case (cf. section 5). As a further consequence Ω^1 is free with dual basis $\mathrm{d}t$, $\mathrm{d}\xi^i$, $i = 1, \ldots, 2n$, and hence

$$\mathrm{d}f = \mathrm{d}t \, \hat{\partial}_t f + \mathrm{d}\xi^i \, \partial_i f \ . \tag{4.13}$$

Using the bilinear form b we define a linear mapping from Ω^1 to $\mathcal{X}$, $\alpha \mapsto \alpha^b$ by

$$\langle \alpha^b, \beta \rangle := b(\alpha, \beta) \ .$$

Note that $(\mathrm{d}t)^b = 0$ and $(\mathrm{d}\xi^i)^b = b^{ij} \partial_j$.

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Relations for forms of higher grade are obtained by applying d on equations (4.4), (4.5). We find

$$\mathrm{d}\xi^i\mathrm{d}\xi^j + \mathrm{d}\xi^j\mathrm{d}\xi^i = \mathrm{d}t\mathrm{d}b^{ij} \,,$$
$$\mathrm{d}t\mathrm{d}t = 0 \,, \qquad \mathrm{d}\xi^i\mathrm{d}t + \mathrm{d}t\mathrm{d}\xi^i = 0 \,. \tag{4.14}$$

These are special cases of

$$\mathrm{d}f\mathrm{d}g + \mathrm{d}g\mathrm{d}f = \mathrm{d}t\,\mathrm{d}b(\mathrm{d}f,\mathrm{d}g) \,, \tag{4.15}$$

which is obtained by application of d on (4.6).

From (4.6) and (4.15) follows that all deviations of the present differential calculus from the classical differential calculus are proportional to dt. Therefore and by the second equation in (4.14) it is also clear that for forms dtϕ, for any $\phi \in \Omega$ all calculations proceed classically. This will help us to proceed more rapidly in what follows.

We extend the $\bullet$ product to act between any 1-form α and an arbitrary form ϕ by using the "insert" opeartor $\lrcorner$ of ordinary exterior calculus

$$\alpha \bullet \phi := \mathrm{d}t\,\alpha^b \lrcorner \phi \,. \tag{4.16}$$

On the right hand side everything is as in the ordinary differential calculus because of the presence of dt . It is not difficult to see that (cf. (4.2))

$$\mathrm{d}f \bullet \phi = [\phi, f] \,.$$

For a one form α the combination $\alpha\bullet$ acts as a derivation of the product of differential forms, i.e.

$$\alpha \bullet (\phi\psi) = (\alpha \bullet \phi)\psi + \phi(\alpha \bullet \psi) \,.$$

The elements u of $\mathcal{X}$ which vanish on t, i.e. $u(t) = 0$ are derivations of $\mathcal{A}$ and define a left $\mathcal{A}$ submodule $\mathcal{X}_1$ of $\mathcal{X}$. With every $u \in \mathcal{X}_1$ we associate mappings $D_u : \Omega \to \Omega$ defined up to terms lying in d$t\,\Omega$ through the following relations

$$D_u(\phi\psi) = (D_u\phi)\psi + \phi(D_u\psi) \quad (\mathrm{mod}\ \mathrm{d}t) \,, \tag{4.17}$$

$$D_u f := u(f) \,, \tag{4.18}$$

and

$$D_u\mathrm{d}t = 0 \quad (\mathrm{mod}\ \mathrm{d}t) \,. \tag{4.19}$$

We write D_i for D_{∂_i} and we set

$$D_i\mathrm{d}\xi^j = -\mathrm{d}\xi^k\,{}^j{}_{ki} \quad (\mathrm{mod}\ \mathrm{d}t) \,, \tag{4.20}$$

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for the coefficients of the connection. For an r-form ϕ with

$$\phi = \frac{1}{r!}\phi_{i_1\cdots i_r}\mathrm{d}\xi^{i_1}\cdots\mathrm{d}\xi^{i_r} \quad (\text{mod } \mathrm{d}t)\ ,$$

we find

$$D_k\phi = \frac{1}{r!}\nabla_k\phi_{i_1\cdots i_r}\mathrm{d}\xi^{i_1}\cdots\mathrm{d}\xi^{i_r} \quad (\text{mod } \mathrm{d}t)\ , \tag{4.21}$$

where

$$\nabla_k\phi_{i_1\cdots i_r} := \partial_k\phi_{i_1\cdots i_r} - {,}^{j}_{\ ki_1}\phi_{j\cdots i_r} - \cdots - {,}^{j}_{\ ki_r}\phi_{i_1\cdots j}\ . \tag{4.22}$$

Extending these definitions as usual to tensor products we obtain

$$\nabla_i b^{jk} := \partial_i b^{jk} + b^{\ell(j,\ ^{k)}}{}_{\ell i};\ . \tag{4.23}$$

In the following *we demand the connection to be torsion free i.e.* ${,}^{i}_{\ [jk]} = 0$, from which follows

$$\mathrm{d}\phi = \mathrm{d}\xi^i\, D_i\phi \quad (\text{mod } \mathrm{d}t)\ , \tag{4.24}$$

and *b-compatible*, that is $\nabla_i b^{jk} = 0$.

It should be emphasized here that in the context of the present noncommutative differential calculus it is possible to develop systematically tensor analysis so that the introduction of the above mentioned concepts of a connection and covariant derivative (cf. eqs(4.17)–(4.20), (4.21)–(4.23)) is made perfectly rigorous. However, this would lead us far away from our task to develop symplectic geometry and Hamiltonian dynamics and therefore it will be presented in a subsequent paper. Let us also remark here that in the old-fashioned index notation these differential geometric tools are first introduced in [41].

With the aid of these mappings and the $\bullet$ we define a new product in Ω

$$\phi \wedge \psi := \phi\psi + (D_i\phi)(\mathrm{d}\xi^i \bullet \psi)\ . \tag{4.25}$$

It is easy to check that $\wedge$ is right $\mathcal{A}$ linear in both factors, i.e.

$$(\phi f) \wedge (\psi g) = (\phi \wedge \psi)fg\ . \tag{4.26}$$

Furthermore it can be shown that the product is associative and as we shall see below also graded commutative, i.e. for $\phi \in \Omega^r$ and $\psi \in \Omega^s$

$$\phi \wedge \psi = (-1)^{rs}\psi \wedge \phi\ .$$

An easy consequence of the above definition is

$$\phi \wedge f = \phi f\ , \qquad\qquad f \wedge \phi = f\phi + \mathrm{d}f \bullet \phi = \phi f\ .$$

We define now an operator

$$\mathrm{D}f := \mathrm{d}f + \frac{1}{2}\mathrm{d}\xi^i \bullet D_i \mathrm{d}f \; , \tag{4.27}$$

motivated by the fact that it satisfies the usual Leibniz rule

$$\mathrm{D}(fg) = (\mathrm{D}f)g + (\mathrm{D}g)f$$

Note that because of this property the 1-forms

$$\mathrm{D}\xi^i := \mathrm{d}\xi^i - \frac{1}{2}\mathrm{d}t,^i \; , \tag{4.28}$$

transform right-covariantly under a change of coordinates $\xi'^j = \xi'^j(\xi)$, i.e. we have $\mathrm{D}'\xi'^j = \mathrm{D}\xi^i\,(\partial_i\xi'^j)$. Here we have set $,^i := b^{jk},^i{}_{jk}$. Clearly $\mathrm{d}t, \mathrm{D}\xi^1,\ldots,\mathrm{D}\xi^{2n}$ form a basis of Ω^1 with

$$\mathrm{D}f = \mathrm{D}\xi^i(\partial_i f) + \mathrm{d}t(\partial_t f) \; ,$$

and

$$\begin{aligned}
\mathrm{d}f &= \mathrm{D}f - \frac{1}{2}\mathrm{d}t\, b^{ij}\nabla_i\partial_j f \; , \\
&= \mathrm{D}\xi^i(\partial_i f) + \mathrm{d}\xi^i(\tilde{\partial}_t f) \; ,
\end{aligned} \tag{4.29}$$

where

$$\tilde{\partial}_t f := \partial_t f - \frac{1}{2}b^{ij}\nabla_i\partial_j f \; . \tag{4.30}$$

The vector fields $\tilde{\partial}_t, \partial_1,\ldots,\partial_{2n}$ form a basis of $\mathcal{X}$ dual to the above basis of Ω^1. From the definitions we find

$$\mathrm{D}\xi^i\mathrm{D}\xi^j = \mathrm{d}\xi^i\mathrm{d}\xi^j + \frac{1}{2}\mathrm{d}t\mathrm{d}\xi^{[i,\; j]} \; , \tag{4.31}$$

$$\mathrm{D}\xi^i \wedge \mathrm{D}\xi^j = \mathrm{D}\xi^i\mathrm{D}\xi^j + \mathrm{d}t\mathrm{d}\xi^k\, b^{\ell j},^i{}_{k\ell} \; , \tag{4.32}$$

and using (4.14) we obtain

$$\begin{aligned}
\mathrm{D}\xi^i \wedge \mathrm{D}\xi^j + \mathrm{D}\xi^j \wedge \mathrm{D}\xi^i = 0 \; , \\
\mathrm{d}t \wedge \mathrm{D}\xi^i = \mathrm{d}t\mathrm{d}\xi^i \; , \qquad \mathrm{D}\xi^i \wedge \mathrm{d}t = \mathrm{d}\xi^i\mathrm{d}t \; , \qquad \mathrm{d}t \wedge \mathrm{d}t = \mathrm{d}t\mathrm{d}t = 0 \; .
\end{aligned} \tag{4.33}$$

It is now easy to see using (4.26) and (4.33), that $\wedge$ is antisymmetric. With the aid of the curvature of the connection $,\,,$

$$R^i{}_{jk\ell} := \partial_k,^i{}_{j\ell} - \partial_\ell,^i{}_{jk} + ,^i{}_{mk},^m{}_{j\ell} - ,^i{}_{m\ell},^m{}_{jk} \; ,$$

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and the curvature 2-form

$$\Omega^i{}_j := \frac{1}{2} R^i{}_{jk\ell} \mathrm{d}\xi^k \mathrm{d}\xi^\ell \quad (\mathrm{mod}\ \mathrm{d}t)\ ,$$

we can prove the following usefull formulae

$$D_{[i} D_{j]} \phi = -R^k{}_{\ell ij} \mathrm{d}\xi^\ell (\partial_k \lrcorner \phi) \quad (\mathrm{mod}\ \mathrm{d}t)\ ,$$

$$\mathrm{d}D_i\phi - D_i\mathrm{d}\phi = -\Omega^j{}_i(\partial_j \lrcorner \phi) + \mathrm{d}\xi^j,\ {}^k{}_{ij} D_k\phi \quad (\mathrm{mod}\ \mathrm{d}t)\ ,$$

and

$$\mathrm{d}(\mathrm{d}\xi^i \bullet \phi) - \mathrm{d}\xi^i \bullet \mathrm{d}\phi = -\mathrm{d}t\, b^{ij} D_j\phi - \mathrm{d}\xi^j,\ {}^i{}_{jk}(\mathrm{d}\xi^k \bullet \phi)\ .$$

Using these one can prove (see also [29] §7) for $\phi \in \Omega^r$ and $\psi \in \Omega$

$$\mathrm{d}(\phi \wedge \psi) = (\mathrm{d}\phi) \wedge \psi + (-1)^r \phi \wedge (\mathrm{d}\psi) + \Omega^j{}_i(\partial_j \lrcorner \phi)(\mathrm{d}\xi^i \bullet \psi) + \mathrm{d}t\, b^{ij}(D_i\phi)(D_j\psi)\ . \quad (4.34)$$

A special case of this formula is

$$\mathrm{d}(\phi f) = (\mathrm{d}\phi)f + (-1)^r \phi \wedge \mathrm{d}f + \mathrm{d}t\, b^{ij}(D_i\phi)(\partial_j f)\ . \quad (4.35)$$

For a 1-form $\alpha = \mathrm{D}\xi^i \alpha_i + \mathrm{d}t \alpha_t$ we find using (4.34)

$$\mathrm{d}\alpha = \frac{1}{2}\mathrm{D}\xi^i \wedge \mathrm{D}\xi^j\, \partial_{[i}\alpha_{j]} + \mathrm{d}t\mathrm{d}\xi^i \left[\partial_t \alpha_i - \partial_i \alpha_t - \frac{1}{2} b^{jk}(\nabla_j \nabla_k \alpha_i + R^\ell{}_{jki}\alpha_\ell) \right]\ .$$

To connect the above results to symplectic geometry and Hamiltonian dynamics we need the exterior derivative of a 2-form ω. In general

$$\omega = \frac{1}{2}\mathrm{D}\xi^i \wedge \mathrm{D}\xi^j\, \omega_{ij} + \mathrm{d}t\mathrm{d}\xi^i \omega_i\ ,$$

(see (4.33) and the remark before (4.29)). Then a lengthy calculation gives

$$\begin{aligned}
\mathrm{d}\omega &= \frac{1}{3!}\mathrm{D}\xi^i \wedge \mathrm{D}\xi^j \wedge \mathrm{D}\xi^k \left[\frac{1}{2}\partial_{[i}\omega_{ik]}\right] + \\
&\quad \frac{1}{2}\mathrm{d}t\mathrm{d}\xi^i\mathrm{d}\xi^j \left[\partial_t\omega_{ij} - \partial_{[i}\omega_{j]} - \frac{1}{2}b^{k\ell}(\nabla_k\nabla_\ell\omega_{ij} - R^m{}_{k\ell[i}\omega_{j]m} - R^m{}_{kij}\omega_{\ell m})\right]\ .(4.36)
\end{aligned}$$

Therefore a 2-form ω is closed, if

$$\partial_{[i}\omega_{jk]} = 0\ , \quad (4.37)$$

and

$$\partial_t\omega_{ij} - \partial_{[i}\omega_{j]} - \frac{1}{2}b^{k\ell}(\nabla_k\nabla_\ell\omega_{ij} - R^m{}_{k\ell[i}\omega_{j]m} - R^m{}_{kij}\omega_{\ell m}) = 0\ . \quad (4.38)$$

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If we now assume as in ordinary symplectic mechanics, that $\partial_t \omega_{ij} = 0$ then it can be proved that (4.37), (4.38) imply that ω_i satisfies

$$\partial_{[i}(\omega_{j]} + \frac{1}{2} b^{k\ell} \nabla_{|k} \omega_{\ell|j]}) = 0 \, , \tag{4.39}$$

where only i, j are antisymmetrized. Therefore ω takes the form

$$\omega = \frac{1}{2} \mathrm{D}\xi^i \wedge \mathrm{D}\xi^j \, \omega_{ij} + \mathrm{d}t\mathrm{d}\xi^i (\partial_i H - \frac{1}{2} b^{k\ell} \nabla_k \omega_{\ell i}) \, ,$$

for some function H. On the other hand (4.37) is the condition for ω_{ij} to be closed in the ordinary exterior calculus, hence by Darboux's theorem it can be brought locally to the form

$$\omega_{ij} = J_{ij} \, , \qquad J = (J_{ij}) = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \, , \qquad I = (\delta_{\alpha\beta}) \, , \quad \alpha, \beta = 1, \dots, n \, ,$$

where J is the symplectic form in canonical coordinates. According to the interpretation of ξ^i in section 5 this can also be assumed in the present context. Therefore, to give our results a more familiar form we write ω in this form

$$\omega = \frac{1}{2} \mathrm{D}\xi^i \wedge \mathrm{D}\xi^j \, J_{ij} + \mathrm{d}t\mathrm{d}\xi^i (\partial_i H - \frac{1}{2} b^{k\ell} \nabla_k J_{\ell i}) \, . \tag{4.40}$$

However the subsequent calculations do not make any use of the fact that ξ^i are taken here to be canonical coordinates.

We already used the "insert" operator $\lrcorner$ in the sense of the classical differential calculus. It is necessary to extend its definition in the present context, since it is needed in the calculation of Hamiltonian vector fields. For $X \in \mathcal{X}$, $f \in \mathcal{A}$ it is natural to put $X \lrcorner f = 0$ and as in the ordinary exterior calculus we set

$$\begin{aligned} X \lrcorner \alpha &:= \langle X, \alpha \rangle \, , \\ X \lrcorner (\phi \wedge \psi) &:= (X \lrcorner \phi) \wedge \psi + (-1)^r \phi \wedge (X \lrcorner \psi) \, , \end{aligned} \tag{4.41}$$

for $\alpha \in \Omega^1$, $\phi \in \Omega^r$ and $\psi \in \Omega$. If $X = X^i \partial_i + X^t \tilde{\partial}_t$ in the coordinate system in which ω has the form (4.40), we have $X \lrcorner \mathrm{D}\xi^i = X^i$ and $X \lrcorner \mathrm{d}t = X^t$. Therefore we find that

$$X \lrcorner \omega = \mathrm{D}\xi^i \left[-J_{ij} X^j + X^t (\partial_i H + F_i) \right] + \mathrm{d}t X^i (\partial_i H + F_i) \, , \tag{4.42}$$

$$F_i := -(1/2) b^{jk} \nabla_j J_{ki} \, . \tag{4.43}$$

In order to write ω in the form (4.40), it is necessary that it has maximal rank, which is $2n$ since $M \times \mathbb{R}$ is odd-dimensional. Therefore it has a 1-dimensional kernel given by the relation

$$X \lrcorner \omega = 0 \, . \tag{4.44}$$

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In ordinary extended Hamiltonian mechanics H is the Hamiltonian[12] and the kernel is identified by definition with the space of Hamiltonian vector fields X.

Equations (4.42), (4.44) give

$$J_{ij}X^j = X^t(\partial_i H + F_i) , \qquad X^i(\partial_i H + F_i) = 0 . \qquad (4.45)$$

Setting $J^{ij} := J_{ij}$ we have $J^{ik}J_{jk} = \delta^i_j$ hence the first equation gives

$$X^i = -X^t J^{ij}(\partial_j H + F_j) ,$$

and consequently the 2nd equation is identically satisfied. Therefore the Hamiltonian vector field defined by H is given by

$$X = X^t \left((\partial_i H + F_i)J^{ij}\partial_j + (\partial_t - \frac{1}{2}b^{ij}\nabla_i\partial_j) \right) . \qquad (4.46)$$

As in ordinary extended Hamiltonian dynamics, the equation of motion for an observable A, i.e. for $A \in \mathcal{A}$ takes the form $X A = 0$, which gives

$$\partial_t A = - \left[\{H, A\} + F_i J^{ij}\partial_j A \right] + \frac{1}{2}\partial_i(b^{ij}\partial_j A) + \frac{1}{2}b^{ij}, {}^k{}_{ki}\partial_j A . \qquad (4.47)$$

The *Hamiltonian equation* is now identical with the general kinetic equation (2.5) for a classical open system in interaction with a large bath at canonical equilibrium, provided that

$$\alpha^{ij} = \frac{1}{2}b^{ij} , \qquad (4.48a)$$

$$F_i = \partial_i F , \qquad (4.48b)$$

$$, {}^k{}_{ki} = -\beta\partial_i H , \qquad (4.48c)$$

with $\{F, H\} = 0$.

Condition (4.48b) is equivalent to $\partial_{[i}F_{j]} = 0$ which by (4.38), (4.39), (4.43) takes the form

$$b^{k\ell}(\nabla_k\nabla_\ell J_{ij} - R^m{}_{k\ell[i}J_{j]m} - R^m{}_{kij}J_{\ell m}) = 0 . \qquad (4.49)$$

When b^{ij} is nondegenerate, this is equivalent to the condition that the *symplectic form J_{ij} is harmonic with respect to the Laplace-Beltrami operator of b* (see e.g. [35] p.3). Equation (4.48c) is equivalent to the condition that the canonical measure

$$\epsilon = e^{-\beta H}\mathrm{d}\xi^1 \cdots \mathrm{d}\xi^{2n} \quad (\mathrm{mod}\ \mathrm{d}t) , \qquad (4.50)$$

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[12]Notice that by (4.31), (4.32), eq.(4.40) is $\omega = (1/2)\mathrm{d}\xi^i\mathrm{d}\xi^j J_{ij} + \mathrm{d}t\mathrm{d}\xi^i\partial_i H$, strongly reminding conventional extended Hamiltonian dynamics.

is covariantly constant $D_i \epsilon = 0$ (see e.g. [36] p.215).

The above results can now be summarized by saying that if the phase-space of a classical open system Σ is endowed with a noncommutative geometrical structure (4.4), (4.5), because of its interaction with a bath at canonical equilibrium, then the corresponding *Hamiltonian* evolution of observables is identical to that given by conventional kinetic theory *if* the symplectic form is "harmonic" with respect to the "metric" connection defined by b^{ij}, and the canonical (Maxwell-Boltzmann) measure defined on Σ at the bath temperature is covariantly constant. Condition (2.3) is not expected to follow from the procedure followed so far, unless a precise relation of (4.4), (4.5) to conventional dynamics is somehow made plausible. This will be considered in another paper.

5 Discussion

In the previous section we have given geometric conditions so that Hamiltonian dynamics in the context of noncommutative differential calculus defined on $M \times \mathbb{R}$ by (4.4)-(4.6) can be interpreted physically as kinetic theory of classical open systems interacting with a large bath at canonical equilibrium.

As already remarked at the end of section 3 the presentation so far is formal in the sense that the nature of the algebra $\mathcal{A}$ and its corresponding coordinate representation in terms of ξ^i has not been specified. Here we discuss these questions further, but it should be emphasized that this is not done rigorously. Actually much remains to be done for the complete clarification of the problems addressed in this section.

At the beginning of section 4 we remarked that a 1-form α in the universal differential envelope of the algebra of functions on a set N is a function $\alpha : N \times N \to \mathbb{C}$ obtained by the obvious extension of (4.1), that is of

$$(f \tilde{\mathrm{d}} g\, h)(a,b) = f(a)[g(b) - g(a)]h(b) . \tag{5.1}$$

For the $\tilde{\bullet}$ we can show that (5.1) implies

$$(\tilde{\mathrm{d}} f_1 \tilde{\bullet} \cdots \tilde{\bullet} \tilde{\mathrm{d}} f_r)(a,b) = (f_1(b) - f_1(a)) \cdots (f_r(b) - f_r(a)) . \tag{5.2}$$

Relations like $\alpha \tilde{\bullet} \beta - \tilde{\mathrm{d}} t\, \tilde{b}(\alpha, \beta) = 0$ are in general incompatible with the above prescription of evaluating differential forms. Therefore if we do impose such relations (i.e. pass from $(\tilde{\Omega}, \tilde{\mathrm{d}}, \tilde{\bullet})$ to $(\Omega, \mathrm{d}, \bullet)$ as it is outlined at the beginning of section 4) *and* at the same time we still want to retain somehow an interpretation of $\bullet$, similar to that given by (5.2) then the elements of Ω^1 cannot be functions on the whole of $N \times N$. In fact such relations induce some structure on $N \times N$ by grouping together points of N which may be considered as neighbouring. This is best illustrated by giving some examples.

Take $N := \mathbb{R}$ the real line. Let x be the coordinate function on N and impose the relation $\mathrm{d}x \bullet \mathrm{d}x - \mathrm{d}x = 0$ (cf. [42]). If we want to keep the interpretation of one forms

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as functions on some set N_1, this cannot be the whole of $N \times N$. It is obvious that N_1 must be that subset of $N \times N$ on which the imposed condition is satisfied identically. If $(a, b) \in N_1 \subset N \times N$ then since $x(a) = a$ we find

$$0 = (\mathrm{d}x \bullet \mathrm{d}x - \mathrm{d}x)(a, b) = (b - a)(b - a - 1) \ .$$

Hence in order for (a, b) to be an element of N_1 either $b = a$ or $b = a + 1$. Hence $N_1 = \{(a, a), (a, a + 1) | \, a \in \mathbb{R}\}$. This set gives a structure on the set N by specifying which of its points are to be considered as neighbouring. Obviously the above condition specifies a discrete structure on $\mathbb{R}$. The possibility to evaluate a one form on (a, b) with a and b not neighbours is still given, if $b - a = m \in \mathbb{Z}$, and corresponds to the "integral"

$$\int_a^b \alpha := \sum_{k=1}^m \alpha(a + k - 1, a + k) \ .$$

Applying the same reasoning to the relation $\mathrm{d}f \bullet \mathrm{d}g = 0$ with smooth functions $f, g : \mathbb{R} \to \mathbb{C}$, then for $a, b \in \mathbb{R}$ we find

$$(\mathrm{d}f \bullet \mathrm{d}g)(a, b) = (f(b) - f(a)) \, (g(b) - g(a)) = f'(x_1)g'(x_2)(b - a)^2 = 0 \ ,$$

where we have used the mean value theorem. Since this condition must hold for all smooth functions we must have $\epsilon := b - a$ and $\epsilon^2 = 0$. Now this relation gives something trivial since ϵ must identically vanish. But the relation $\mathrm{d}f \bullet \mathrm{d}g = [\mathrm{d}f, g] = 0$ holds in the usual differential calculus and consequently it cannot be trivial. In fact one may interprete relation $\epsilon^2 = 0$ as saying, that ϵ is an infinitesimal of first order. In this sense $\mathbb{R}$ is again structured since now $N_1 := \{(a, a), (a, a+\epsilon) | \, a \in \mathbb{R}\}$. For arbitrary $a < b \in \mathbb{R}$ the integral is defined by

$$\int_a^b \alpha := \lim \sum_{k=1}^m \alpha(x_{k-1}, x_k) \ , \tag{5.3}$$

where this is obtained by taking the limit of vanishing width of the partition $a = x_0 < x_1 < \cdots < x_m = b$ of $[a, b]$. Now the relation $\mathrm{d}f \bullet \mathrm{d}g = 0$ integrated over $[a, b]$ for arbitrary $a < b \in \mathbb{R}$ gives

$$0 = \int_a^b \mathrm{d}f \bullet \mathrm{d}g = \lim \sum_{k=1}^m (f(x_k) - f(x_{k-1})) \, (g(x_k) - g(x_{k-1})) \ , \tag{5.4}$$

which can be expressed by saying that the "quadratic variation" of functions must vanish. This is true *if* f, g are of bounded variation, a condition which is *necessary* for the Riemann-Stieltjes integral $\int_a^b g \mathrm{d}f$ to exist.

For a second order calculus on smooth functions of one variable ξ, parametrizing $N := \mathbb{R}$, we have by definition (section 4, eq.(4.7)) that $\mathrm{d}f \bullet \mathrm{d}g \bullet \mathrm{d}h = 0$, hence by

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applying $d\xi \bullet d\xi \bullet d\xi = 0$ on $(a, b) \in \mathbb{R}^2$ we get $(\xi(b) - \xi(a))^3 = 0$. Thus $\xi(b) - \xi(a)$ is an infinitesimal of *second* order. Therefore $N_1 = \{(a, a), (a, a + \epsilon), (a, a + \epsilon^2) | a \in \xi^{-1}(\mathbb{R})\}$, in this case and consequently for given $a \in N$ we can move away from a in two ways, either to $a + \epsilon$ or to $a + \epsilon^2$. In this sense then N becomes structured and can be considered as 2-dimensional.[13]

For $a < b \in \mathbb{R}$ we define formally an integral as in (5.2). Applying this on $d\xi \bullet d\xi \bullet d\xi = 0$ we obtain

$$\lim \sum_{k=1}^{m} \left(\xi(x_k) - \xi(x_{k-1}) \right)^3 = 0 \ , \tag{5.5}$$

where again the limit is obtained as in (5.3). This relation can be expressed by saying that the "cubic variation" of ξ must vanish. It is perhaps of independent mathematical interest to find equivalent characterizations of such functions.

Since the quadratic variation of ξ does not vanish in general, ξ cannot be the usual coordinate function of $\mathbb{R}$. Consequently we have $\mathbb{R}$ as a differentiable manifold but with a differential structure which is not the standard one. If we set $dt := (1/b)d\xi \bullet d\xi$ with some constant b and t a function on $\mathbb{R}$, then by (2.5) $dt \bullet dt = 0$ and hence t is of bounded variation and can be taken to be the coordinate function on some copy of $\mathbb{R}$. This additional coordinate t realizes somehow the fact that N is 2-dimensional.

In the light of the above remark, if $M = \mathbb{R}^{2n}$, it seems that ξ^i should be interpreted as local coordinates defined on $\mathbb{R}^{2n}$ by an atlas $\hat{\mathcal{U}}$ not compatible with the usual one giving the standard differential structure of $\mathbb{R}^{2n}$; that is there are charts in $\hat{\mathcal{U}}$ not C^k-related to the identity mapping of $\mathbb{R}^{2n}$, for some $k > 0$. Equivalently we may say that the identity mapping of $\mathbb{R}^{2n}$, does not belong to $\hat{\mathcal{U}}$. More generally, for a $2n$-dimensional differentiable manifold M the above discussion implies that if ξ is a local chart of M in $\mathbb{R}^{2n}$ and $\hat{\xi}$ a local chart of $\mathbb{R}^{2n}$ from $\hat{\mathcal{U}}$ the functions $f : M \to \mathbb{C}$ belonging to $\mathcal{A}$, are smooth functions of ξ but are not smooth, not even of bounded variation, as functions of $\hat{\xi}$, that is $f \circ \xi^{-1}$ are smooth, but $f \circ (\hat{\xi} \circ \xi)^{-1}$ are not.

The whole discussion in this section reminds us strongly of stochastic calculus on manifolds developed in the context of semimartingale theory, in particular when stochastic terms are given in terms of Wiener processes (see e.g. [37], [38]). In fact there are many results in stochastic calculus having an exact analogue in the formalism developed here. As examples compare (4.8) with (4) in [38] p.134 and their properties, or elements of $\mathcal{X}$ eq.(4.10) with the characterization of 2nd order fields in [38] Lemma 6.1. Moreover our relation of the "metric connection" with the drift term in the general Fokker-Planck type kinetic equation (4.43) suggests a close relation with the interpretation in stochastic calculus of a connection on a manifold as a mapping giving the "drift" of a 2nd order vector field ([37] p.258–259).In fact it seems possible — and it will be examined elsewhere

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[13]The equality $N = \mathbb{R}$ is only set-theoretic.

— that our present model of noncommutative geometry can be realized in the context of stochastic calclulus. However, whether this is the only possibility remains an interesting, but to our knowledge, still unsolved problem.

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