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 of at most second order. For open systems interacting with a bath at canonical equilibrium they have the 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 that certain conditions, geometric in character, are fulfilled. To this end, symplectic geometry on M is developed in this context, and an outline of the required tensor analysis and differential geometry is given. Certain questions as regards the possible mathematical interpretation of this structure are also discussed.

1. Introduction

Achieving an understanding and description of the 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 viewpoint 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 argument methods, based on some presumably plausible assumptions on the behaviour of a large number of microscopic events characterizing the system;

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

Typical examples for (i) are the Fokker–Planck and Kramers equations (see, 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, and the second refers to the p.d.f. of its phase-space position in the presence of an external field. The basic assumptions for their derivations are that the microscopic dynamics of

the Brownian particle are governed by Langevin's equation and that its p.d.f. is that of a Markovian diffusion process (see, e.g., [2], ch II, and [3]). This procedure usually leads to *model* equations that are easier to study than the equations that are *assumed* to be more fundamental following from exact dynamics via (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 (see, e.g., [4], ch 4, and [5], ch 9). Though these points are interesting and important from both the mathematical and physical point of view, it seems that one has to know somehow the kinetic equation that one 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 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) and 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 their equivalent, the BBGKY hierarchy of equations truncated on the basis of physical considerations†.

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 when one tries to extend it to other systems and/or a higher order of approximation* ([12]; [13], section 5). For instance the linearized Landau equation follows for spatially homogeneous plasmas as a second-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 a higher order of approximation and/or for inhomogeneous systems, runs into difficulties (e.g. equations violating the positivity of the p.d.f. or having no H-theorem are obtained— see, e.g., [14] in connection with [13], section 5), or involves highly *ad hoc* steps which are sometimes hidden in the calculations (see, e.g., [15] in connection with section 2 below).

Although one may be tempted to accept that there is no reason to expect equations in an approximate theory to share all the 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, the 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!‡

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

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† See, e.g.: [6], sections 30, 41; [7], ch 20; [8], ch IX; [9], section 2.4; [10], sections 4.3, 4.6; [11], section VI.
‡ See, e.g., equations following from expansion of Liouville's equation or the so-called generalized master equation ([10], section 2.3; [12], section 2; [13], section 5; [27]) in connection with the last paragraph of the next section. See also [34] for expansions of the Boltzmann equation.

or quantum) *reversible dynamics*. To put it differently, the *aim* of kinetic theory (the 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 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 there lies a probabilistic interpretation. Using this as a motivation and in order to clarify the difficulties mentioned in the previous section, 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 *classical* systems, though similar results are known for quantum systems as well ([19], and [16], theorem 4.2).

We make the following assumptions.

(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 (see, e.g., [21], pp 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 a 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 properties 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†.

(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 regular probability Borel measure on M (see, e.g., [23], p 399, and [24], theorem 2.1, for an outline of a proof). If we further *assume* that M is an n-dimensional differential manifold, that the generator of the semigroup is defined on C^2-functions and that a Lindenberg-type condition holds,

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

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

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) has the form†

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

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 in the following work‡. 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

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

where $\{\ ,\ \}$ is 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§. 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 non-rigorous language) that *linear autonomous kinetic equations for classical systems, which are differential equations, are necessarily of at most second order with non-negative-definite leading coefficients and vanishing zeroth-order terms* (cf. equation (2.1))‖.

Since kinetic equations following from microscopic dynamics (see section 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¶. In the rest of this paper, we will present a different point of view, motivated by the discussion in the next section.

† See [25], theorem 5.3, for an outline of a proof, and [26], theorem XIII.53, for a partial generalization—the Lévy–Khinchine formula.
‡ For detailed proofs and more precise formulation of the various conditions see [27].
§ See, e.g.: [13], proposition 4.1; [28], equation (2.19); [6], p 190; [18], equations (III.26) and (III.16) together with (III.19); [32], equation (5.8).
‖ A corresponding result is also known for quantum systems [19, 17, 18, 20]. The special case of the Kramers–Moyal expansion of the linearized Boltzmann equation has been considered in [34].
¶ See, e.g., [10], section 2.4, equation (2.199), and [1], p 215, section IX.6—particularly p 280.

3. Non-commutative geometry and stochastic calculus

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

microscopic (Hamiltonian dynamics)
+ $\implies$ kinetic equations.
some systematic approximation scheme

On the other hand, method (i) in section 1 involves no systematic approximation scheme but a modification of the microscopic dynamics which now takes the form of stochastic differential equations. In our opinion, the weak point in this case is that there is no general method of choosing the microscopic stochastic differential equations. That is, it seems necessary that one somehow knows the kinetic equation that one 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 differential equations in phase space involving Wiener processes X_t of the form

$$\begin{pmatrix} \mathrm{d}\boldsymbol{q} \\ \mathrm{d}\boldsymbol{p} \end{pmatrix} = \begin{pmatrix} \boldsymbol{A}_q(\boldsymbol{q}, \boldsymbol{p})\,\mathrm{d}t + \boldsymbol{F}_q(\boldsymbol{q}, \boldsymbol{p}) \cdot \mathrm{d}\boldsymbol{X}_t^q \\ \boldsymbol{A}_p(\boldsymbol{q}, \boldsymbol{p})\,\mathrm{d}t + \boldsymbol{F}_p(\boldsymbol{q}, \boldsymbol{p}) \cdot \mathrm{d}\boldsymbol{X}_t^p \end{pmatrix} \tag{3.1}$$

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

In the following sections we outline *another approach* in which *the Hamiltonian character of microscopic dynamics is retained but, instead of approximation schemes, we make the fundamental assumption that observables are now defined on a manifold with non-commutative geometrical structure*. As will be explained, this may be interpreted as a stochastic dynamical structure, though it is not known whether or not this is necessary. Nevertheless, the formulation developed in the next section is closely related to what may be called a differential geometric approach to stochastic calculus†, though this relation will be further explored in another paper.

The *mathematical* motivation for introducing non-commutative 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 of differential forms spanned by $\mathrm{d}t$, $\mathrm{d}X_t$ 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 second derivatives in Itô's formula for the differential of such functions ([29], section 2—particularly equation (2.4)). However, it is possible to define a modified *non-commutative* but still associative product of functions and differential forms such that Leibniz's rule holds ([29], section 3, [31]). This product induces a non-commutative 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:

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

where γ is the diffusion constant appearing in the usual Fokker–Planck equation obtained from Langevin's equation ([29], equation (3.16)). Equation (3.2) is readily generalized to a

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

multidimensional Wiener process:

$$[dt, t] = [dt, X_t^i] = 0 \qquad [dX_t^i, X_t^j] = b^{ij} \ dt \qquad (3.3)$$

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

$$[df, g] = b(df, dg) \ dt \qquad (3.4)$$

for functions f, g of $\boldsymbol{X}_t, t$ and a symmetric, bilinear form with components b^{ij} in the 'coordinates' X_t^i and such that dt 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 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 an 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‡. 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 whether or not others exist. A preliminary discussion of this problem is given in section 6.

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

4. Non-commutative 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 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

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† This is implied by the fact that since d satisfies Leibniz's rule, $[dX_t^i, X_t^j] = [dX_t^j, X_t^i]$, which in fact shows that this commutator depends only on dX_t^i, dX_t^j—see [30], section 3.
‡ For details on the systematic definition and presentation of general results in non-commutative geometry on a commutative algebra, see [30], particularly sections 2 and 3.

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

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

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

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

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

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

and hence $\tilde{\mathrm{d}}f\, g \neq g\, \tilde{\mathrm{d}}f$. On the $\mathcal{A}$-bimodule of 1-forms $\tilde{\Omega}^1$ we define a new product $\tilde{\bullet}\colon \tilde{\Omega}^1 \times \tilde{\Omega}^1 \to \tilde{\Omega}^1$ 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 $[\tilde{\mathrm{d}}f, g] = \tilde{\mathrm{d}}f \,\tilde{\bullet}\, \tilde{\mathrm{d}}g$. The universality of $(\tilde{\Omega}, \tilde{\mathrm{d}})$ is expressed by the property that, if (Ω, d) is any differential algebra on $\mathcal{A}$, then there is a graded-algebra homomorphism $\pi\colon \tilde{\Omega} \to \Omega$ of grade 0 such that $\pi|\tilde{\Omega}^0 = \mathrm{id}_{\mathcal{A}}$ and $\mathrm{d} \circ \pi = \pi \circ \tilde{\mathrm{d}}$ (cf. [30], section 3.1).

Let $\tilde{b}\colon \tilde{\Omega}^1 \times \tilde{\Omega}^1 \to \mathcal{A}$ 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 $\tilde{\mathrm{d}}t$ lies in the kernel of $\tilde{b}$. Also let $\mathcal{I}$ denote the differential ideal of $\tilde{\Omega}$ generated by $\alpha \,\tilde{\bullet}\, \beta - \tilde{\mathrm{d}}t\, \tilde{b}(\alpha, \beta)$, then we set $\Omega := \tilde{\Omega}/\mathcal{I}$ and $\pi\colon \tilde{\Omega} \to \Omega$ for the canonical projection. Since $\mathcal{I}$ is a differential ideal the operator $\mathrm{d}\colon \Omega \to \Omega$ given by $\mathrm{d} = \pi \circ \tilde{\mathrm{d}}$ is well defined, and because $\tilde{\mathrm{d}}t$ lies in the kernel of $\tilde{b}$, a symmetric left–right $\mathcal{A}$-bilinear form $b\colon \Omega \times \Omega \to \mathcal{A}$ is uniquely defined by $b \circ (\pi \times \pi) = \tilde{b}$.

Now set

$$\mathrm{d}f \bullet \mathrm{d}g := [\mathrm{d}f, g] \tag{4.2}$$

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

$$\alpha \bullet \beta = \mathrm{d}t\, b(\alpha, \beta). \tag{4.3}$$

This is just a special case of the general procedure used to relate $(\tilde{\Omega}, \tilde{\mathrm{d}})$ 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 using $\tilde{\bullet}$ on $\tilde{\Omega}^1$ (cf. [30], section 3.2). Let ξ^i, $i = 1, \ldots, 2n$, be local coordinates on M; then the elements of $\mathcal{A}$ can be written locally as functions of t, ξ^i, $i = 1, \ldots, 2n$ (see also section 6). If we set $b^{ij} := b\,(\mathrm{d}\xi^i, \mathrm{d}\xi^j)$ we find the commutation relations (note that $b\,(\mathrm{d}t, \mathrm{d}\xi^i) = b\,(\mathrm{d}\xi^i, \mathrm{d}t) = 0$)

$$[\mathrm{d}\xi^i, \xi^j] = \mathrm{d}t\, b^{ij} \tag{4.4}$$

$$[\mathrm{d}t, t] = [\mathrm{d}t, \xi^i] = [\mathrm{d}\xi^i, t] = 0. \tag{4.5}$$

These are special cases of

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

By using (4.2) and (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 make the definition

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

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 locally, as a left $\mathcal{A}$-module, $\mathcal{X}$ is free with basis given by $\hat{\partial}_t, \partial_1, \ldots, \partial_{2n}$, where

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

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, vector fields satisfying (4.7), i.e. elements of $\mathcal{X}$, are second-order differential operators without constant terms, like (4.12). Thus the name second-order calculus is justified in this case (cf. section 6). As a further consequence, Ω^1 is also free with the 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 $\mathcal{X}$, $\alpha \mapsto \alpha^b$ via

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

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

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

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

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 to (4.6).

From (4.6) and (4.15) it follows that all deviations of the present differential calculus from the classical differential calculus are proportional to $\mathrm{d}t$. *Therefore and by the second equation in (4.14) it is also clear that for forms* $\mathrm{d}t \, \phi$, *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 so that it acts between any 1-form α and an arbitrary form ϕ by using the 'insert' operator $\lrcorner$ 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 ordinary differential calculus because of the presence of $\mathrm{d}t$. It is not difficult to see that (cf. (4.2))

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

For a 1-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 $D_u \colon \Omega \to \Omega$ defined up to terms lying in $dt\ \Omega$ through the following relations:

$$D_u(\phi\psi) = (D_u\phi)\ \psi + \phi\ (D_u\psi) \qquad (\text{mod } dt) \tag{4.17}$$

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

and

$$D_u\ dt = 0 \qquad (\text{mod } dt). \tag{4.19}$$

We write D_i for D_{∂_i} and we set

$$D_i\ d\xi^j = -d\xi^k\ \Gamma^j{}_{ki} \qquad (\text{mod } dt) \tag{4.20}$$

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

$$\phi = \frac{1}{r!}\phi_{i_1\cdots i_r}\ d\xi^{i_1}\cdots d\xi^{i_r} \qquad (\text{mod } dt)$$

we find

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

where

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

Extending these definitions as usual to tensor products we obtain

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

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

$$d\phi = d\xi^i\ D_i\phi \qquad (\text{mod } dt). \tag{4.24}$$

It should be emphasized here that in the context of the present non-commutative 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. equations (4.17)–(4.20), (4.21)–(4.23)) is made perfectly rigorous. However, this would lead us far away from our tasks of developing 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 were first introduced in [41].

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

$$\phi \wedge \psi := \phi\psi + (D_i\phi)\ (d\xi^i \bullet \psi) + \frac{1}{2}\ d\xi^k\ (\nabla_k b^{ij})\ (\partial_i \lrcorner \phi)\ dt\ (\partial_j \lrcorner \psi). \tag{4.25}$$

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 $\psi \in \Omega^s$

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

It is not difficult to show from the above definition that

$$\phi \wedge f = \phi f \qquad f \wedge \phi = f\phi + df \bullet \phi = \phi f.$$

We define now an operator

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

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

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

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 $\Gamma^i := b^{jk}\Gamma^i{}_{jk}$. Clearly $\mathrm{d}t, \mathrm{D}\xi^1, \ldots, \mathrm{D}\xi^{2n}$ form a local basis of Ω^1 with

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

and

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

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 local basis of $\mathcal{X}$ dual to the above basis of Ω^1. From the definitions we find

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

$$\mathrm{D}\xi^i \wedge \mathrm{D}\xi^j = \mathrm{D}\xi^i\ \mathrm{D}\xi^j + \mathrm{d}t\ \mathrm{d}\xi^k\ b^{\ell j}\Gamma^i{}_{k\ell} - \frac{1}{2}\ \mathrm{d}t\ \mathrm{d}\xi^k\ (\nabla_k b^{ij}) \tag{4.32}$$

and using (4.14) we obtain

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

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 Γ,

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

and the curvature 2-form

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

we can prove the following useful formulae

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

$$\mathrm{d}\,\mathrm{D}_i\phi - \mathrm{D}_i\ \mathrm{d}\phi = -\Omega^j{}_i(\partial_j \lrcorner\ \phi) + \mathrm{d}\xi^j\ \Gamma^k{}_{ij}\ \mathrm{D}_k\phi \qquad (\mathrm{mod}\ \mathrm{d}t)$$

$$\pounds_{\partial_i}\phi = \mathrm{d}(\partial_i \lrcorner\ \phi) + \partial_i \lrcorner\ \mathrm{d}\phi = \mathrm{D}_i\phi + \mathrm{d}\xi^k\ \Gamma^j{}_{ik}(\partial_i \lrcorner\ \phi) \qquad (\mathrm{mod}\ \mathrm{d}t)$$

and

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

Using these one can prove (cf. [29], section 7) for $\phi \in \Omega^r$ and $\psi \in \Omega$

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

$$+ \frac{1}{2} \ d\xi^k \ (\nabla_k b^{ij}) \ [(D_i\phi) \ dt \ (\partial_j \lrcorner \psi) + dt \ (\partial_i \lrcorner \phi) \ (D_j\psi)]$$

$$+ \frac{1}{2} \ d\xi^k \ d\xi^\ell \ (\nabla_k \nabla_\ell b^{ij}) \ (\partial_i \lrcorner \phi) \ dt \ (\partial_j \lrcorner \psi). \tag{4.34}$$

A special case of this formula is

$$d(\phi f) = (d\phi)f + (-1)^r \phi \wedge df - dt \ b^{ij} \ (D_i\phi) \ (\partial_j f) - \frac{1}{2} \ dt \ d\xi^k \ (\nabla_k b^{ij}) \ (\partial_i \lrcorner \phi) \ (\partial_j f). \tag{4.35}$$

For a 1-form $\alpha = D\xi^i \ \alpha_i + dt \ \alpha_t$ we find using (4.34)

$$d\alpha = \frac{1}{2} D\xi^i \wedge D\xi^j \ \partial_{[i}\alpha_{j]}$$

$$+ dt \ d\xi^i \left[\partial_t \alpha_i - \partial_i \alpha_t - \frac{1}{2} b^{jk} \ (\nabla_j \nabla_k \alpha_i + R^\ell{}_{jki}\alpha_\ell) - \frac{1}{2} \ (\nabla_i b^{jk}) \ (\nabla_j \alpha_k) \right].$$

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

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

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

$$d\omega = \frac{1}{3!} \ D\xi^i \wedge D\xi^j \wedge D\xi^k \left[\frac{1}{2} \ \partial_{[i}\omega_{jk]} \right] + \frac{1}{2} \ dt \ d\xi^i \ d\xi^j \left[\partial_t \omega_{ij} - \partial_{[i}\omega_{j]} \right.$$

$$\left. - \frac{1}{2} b^{k\ell} \ (\nabla_k \nabla_\ell \omega_{ij} - R^m{}_{k\ell[i}\omega_{j]m} - R^m{}_{kij}\omega_{\ell m}) + \frac{1}{2} \ (\nabla_k \omega_{\ell[i}) \ (\nabla_{j]}b^{k\ell}) \right]. \tag{4.36}$$

Therefore a 2-form ω is closed if

$$\partial_{[i}\omega_{jk]} = 0 \tag{4.37}$$

and

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

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

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

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

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

where J is the symplectic form in canonical coordinates. According to the interpretation of ξ^i in section 6 this can also be assumed in the present context. Therefore, to give our results a more familiar form we write ω in this form:

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

However, the subsequent calculations do not make any use of the fact that the 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

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

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 one-dimensional kernel given by the relation

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

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

Equations (4.42) and (4.44) give

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

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

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

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

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

As in ordinary extended Hamiltonian dynamics, the equation of motion for an observable A, i.e. for $A \in \mathcal{A}$, takes the form $XA = 0$. By noticing that $\nabla_i \partial_j = \partial_i \partial_j - \Gamma^k{}_{ij} \, \partial_k$ and using $J^{ik} J_{jk} = \delta^i_j$ this gives, after some reductions,

$$\partial_t A = - \left[\{H, A\} + \tilde{F}_i J^{ij} \, \partial_j A \right] + \frac{1}{2} \, \partial_i (b^{ij} \, \partial_j A) + \frac{1}{2} b^{ij} \Gamma^k{}_{ki} \, \partial_j A \tag{4.47}$$

where

$$\tilde{F}_i := -\frac{1}{2} \, \nabla_j (b^{jk} J_{ki}). \tag{4.48}$$

† Notice that by (4.31) and (4.32), equation (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 one of conventional extended Hamiltonian dynamics.

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

$$\alpha^{ij} = \frac{1}{2} b^{ij} \tag{4.49a}$$

$$\tilde{F}_i = \partial_i F \tag{4.49b}$$

$$\Gamma^k{}_{ki} = -\beta \; \partial_i H \tag{4.49c}$$

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

In a simply connected phase space, condition (4.49b) is equivalent to $\partial_{[i} \tilde{F}_{j]} = 0$ and takes the form

$$\nabla_{[i} \; \nabla_{|k|} (b^{k\ell} J_{\ell|j]}) = 0. \tag{4.50}$$

To get an insight into the geometric meaning of this condition we may notice that in the case where b^{ij} is non-degenerate and $\Gamma^i{}_{jk}$ its 'metric' connection (i.e. $\nabla_k b^{ij} = 0$), equation (4.50) is equivalent to the condition that the *symplectic form J_{ij} is harmonic with respect to the Laplace–Beltrami operator of b^{ij}* (see, e.g., [35]). However, this is by no means necessary in the context of the present formalism. In fact as will be seen in section 5, b-compatibility of the connection is rather restrictive, ruling out interesting cases of well known kinetic equations. Equation (4.49c) is equivalent to the condition that the canonical measure

$$\epsilon = e^{-\beta H} \; d\xi^1 \cdots \; d\xi^{2n} \quad (\text{mod } dt) \tag{4.51}$$

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 non-commutative geometrical structure, (4.4) and (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 canonical (Maxwell–Boltzmann) measure defined on Σ at the bath temperature is covariantly constant and the symplectic form satisfies a 'generalized harmonic' condition (4.50) (cf. the remark following it). Condition (2.3) is not expected to follow from the procedure followed so far, unless a precise relation of (4.4) and (4.5) to conventional dynamics is somehow made plausible. This will be considered in another paper.

5. Simple applications

Although an attempt to relate the present formalism to conventional dynamics will be made elsewhere, we can easily illustrate our results by showing that well known simple kinetic equations can be incorporated in it. To this end we notice that formally probability density distributions f satisfy the adjoint of (4.47) which under (4.49b) reads

$$\partial_t f = \{H + F, f\} + \frac{1}{2} \; \partial_i (b^{ij} \; \partial_j f - b^{ij} \Gamma^k{}_{kj} f). \tag{5.1}$$

To keep the presentation as simple as possible, we consider one-dimensional systems for which b^{ij} is diagonal and independent of t and $(\xi^1, \xi^2) = (q, p)$, i.e.

$$b^{ij} = \begin{pmatrix} b_1 & 0 \\ 0 & b_2 \end{pmatrix}.$$

Then a simple calculation using (4.48), (4.49*b*), and (4.49*c*) gives

$$\Gamma^2{}_{21} = -\beta\ \partial_q H - \Gamma^1{}_{11} \qquad \Gamma^1{}_{12} = -\beta\ \partial_p H - \Gamma^2{}_{22}$$
$$b_1\Gamma^2{}_{11} = -\partial_q F - b_2\Gamma^2{}_{22} \qquad b_2\Gamma^1{}_{22} = \partial_p F - b_1\Gamma^1{}_{11}. \tag{5.2}$$

By taking account of (2.3) we are left with two unspecified components of the connection, $\Gamma^1{}_{11}$, $\Gamma^2{}_{22}$. When b^{ij} is degenerate but non-zero, e.g. $b_1 = 0$, we still have two unspecified components $\Gamma^1{}_{11}$, $\Gamma^2{}_{11}$. Finally direct application of (4.23) shows that connections satisfying (5.2) are not *b*-compatible in general.

A first example falling into the range of applicability of the above model is the one-dimensional Kramers equation mentioned in section 1, for a classical Brownian particle of mass m in an external field $V(q)$, i.e. with $H = p^2/2m + V$, and

$$\partial_t f = -\frac{p}{m}\ \partial_q f + \partial_q V\ \partial_p f + \gamma\left(\partial_p^2 f + \frac{\beta}{m}\ \partial_p(pf)\right). \tag{5.3}$$

In this case $b_1 = F = 0$, $b_2 = 2\gamma$, so we get

$$\Gamma^2{}_{22} = \Gamma^1{}_{22} = 0 \qquad \Gamma^1{}_{12} = -\beta\frac{p}{m} \qquad \Gamma^2{}_{21} = -\beta\ \partial_q V - \Gamma^1{}_{11} \tag{5.4}$$

whereas $\Gamma^1{}_{11}$, $\Gamma^2{}_{11}$ remain unspecified.

It is well known that quantum kinetic equations can be given a phase-space representation, using various methods. Therefore as a second example we may consider the kinetic equation for a *quantum* oscillator of mass m and frequency ω weakly coupled to a bath of harmonic oscillators at canonical equilibrium with temperature $1/\beta$, which is written in a coherent-state representation (antinormal ordered density matrix) as

$$\partial_t f = (1 - a)\{H, f\} + \frac{2mk}{\beta}\left[\partial_p\ (\partial_p f + \beta pf) + \partial_q\left(\frac{1}{(m\omega)^2}\ \partial_q f + \beta qf\right)\right] \tag{5.5}$$

with $H = p^2/2m + m\omega^2 q^2/2$ and where a, k are ω-independent constants and k has been written to lowest order in $\hbar$, for simplicity†. This equation can be obtained in several ways. The standard one is to apply to this system the general Markovian master equation obtained from the Liouville–von Neumann equation for the system. However, one has to use in this case the rather questionable rotating-wave approximation to the total Hamiltonian to eliminate the so-called antiresonant terms representing simultaneous excitations or de-excitations of the oscillator and some bath oscillator‡. Another more systematic method is that of applying the general formalism of [13] and then passing to a coherent-state representation ([44], ch III E). In fact this equation is the classical limit obtained via a Wigner transformation of a special case of the general Fokker–Planck-type equation, studied in [45]§. Actually it can also be obtained by applying the general formalism of [13] *directly* to the corresponding *classical* Hamiltonian describing a harmonic oscillator coupled to a harmonic chain with nearest-neighbour interactions [47].

In this case

$$b_1 = \frac{k}{\beta m\omega^2} \qquad b_2 = \frac{km}{\beta} \qquad F = -aH.$$

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† See, e.g., [43], equation (6.5.11), p 392, in connection with (6.2.59) and (6.4.37).
‡ See, e.g., [43], sections 6.1, 6.2—particularly p 336 and equation (6.2.34b).
§ Equation (4.5) together with table III; for details see [46], section 6.

Therefore (5.2) gives

$$\Gamma^2{}_{21} = -\beta m\omega^2 q - \Gamma^1{}_{11} \qquad\qquad \Gamma^1{}_{12} = -\frac{\beta}{m}p - \Gamma^2{}_{22}$$

$$\Gamma^2{}_{11} = \frac{\beta a (m\omega^2)^2}{k}q - (m\omega)^2\Gamma^2{}_{22} \qquad \Gamma^1{}_{22} = -\frac{\beta a}{km^2}p - \frac{1}{(m\omega)^2}\Gamma^1{}_{11} \tag{5.6}$$

and once again $\Gamma^1{}_{11}$, $\Gamma^2{}_{22}$ remain unspecified.

We may finally say that in both examples the connection is not flat, even in the case where the above unspecified components of the connection vanish.

6. Discussion

In the previous section we have given geometric conditions so that Hamiltonian dynamics in the context of non-commutative differential calculus defined on $M \times \mathbb{R}$ by (4.4)–(4.6) can be interpreted physically in terms of 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

$$(f \; \tilde{\mathrm{d}}g \; h)(a, b) = f(a)[g(b) - g(a)]h(b). \tag{6.1}$$

For the $\tilde{\bullet}$ we can show that (6.1) implies

$$(\tilde{\mathrm{d}}f_1 \, \tilde{\bullet} \cdots \tilde{\bullet} \, \tilde{\mathrm{d}}f_r) \,(a, b) = (f_1(b) - f_1(a)) \cdots (f_r(b) - f_r(a)). \tag{6.2}$$

Relations like $\alpha \, \tilde{\bullet} \, \beta - \tilde{\mathrm{d}}t \; \tilde{b}(\alpha, \beta) = 0$ are in general incompatible with the above prescription for 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 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 (6.2), 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 1-forms 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 $N \times N$ for 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 of evaluating a 1-form on (a, b) with a and b not neighbours still arises, 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 $f, g \colon \mathbb{R} \to \mathbb{C}$, 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 becomes 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 interpret the relation $\epsilon^2 = 0$ as implying 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

$$\int_a^b \alpha := \lim \sum_{k=1}^m \alpha(x_{k-1}, x_k) \tag{6.3}$$

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

$$0 = \int_a^b \mathrm{d}f \bullet \mathrm{d}g = \lim \sum_{k=1}^m (f(x_k) - f(x_{k-1}))\,(g(x_k) - g(x_{k-1})) \tag{6.4}$$

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, equation (4.7)) that $\mathrm{d}f \bullet \mathrm{d}g \bullet \mathrm{d}h = 0$; hence by applying $\mathrm{d}\xi \bullet \mathrm{d}\xi \bullet \mathrm{d}\xi = 0$ 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 two dimensional†.

For $a < b \in \mathbb{R}$ we define formally an integral as in (6.2) above. Applying this on $\mathrm{d}\xi \bullet \mathrm{d}\xi \bullet \mathrm{d}\xi = 0$ we obtain

$$\lim \sum_{k=1}^m (\xi(x_k) - \xi(x_{k-1}))^3 = 0 \tag{6.5}$$

where again the limit is obtained as in (6.3). 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 $\mathrm{d}t := (1/b)\,\mathrm{d}\xi \bullet \mathrm{d}\xi$ with some constant b and t a function on $\mathbb{R}$, then by (2.5) $\mathrm{d}t \bullet \mathrm{d}t = 0$ 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 two dimensional.

In the light of the above remark, if $M = \mathbb{R}^{2n}$, it seems that the 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 equality $N = \mathbb{R}$ is only set theoretic.

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 $\mathcal{X}$, equation (4.10), with the characterization of second-order fields in [38], lemma 6.1. Moreover our relation of the 'connection' to the drift term in the general Fokker–Planck-type kinetic equation (4.47) suggests a close relation with the interpretation in stochastic calculus of a connection on a manifold as a mapping giving the 'drift' of a second-order vector field ([37], pp 258, 259). In fact it seems possible—and this will be examined elsewhere—that our present model of non-commutative geometry can be realized in the context of stochastic calculus. However, whether this is the only possibility remains an interesting—but to our knowledge, still unsolved—problem.

Acknowledgments

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