

Double bracket formulation for the distribution function approach to multibead-chain suspensions

Ching Lok Chong

11 Feb 2021

OCIAM, Mathematical Institute, University of Oxford, Andrew Wiles Building,
Radcliffe Observatory Quarter, Woodstock Road, Oxford, OX2 6GG, UK

Abstract

A suspension of elastic chains of small beads in a Newtonian fluid is a common model for a viscoelastic polymer solution. The configuration of these multibead chains is described by a distribution function that evolves according to a Liouville or Fokker–Planck equation. The evolution of these multibead-chain suspensions is described using a double bracket formulation with a Hamiltonian functional. The conservative part of the dynamics is described by a Poisson bracket, and the dissipative part by an additional symmetric bracket. We treat the configuration space of multibead chains as a higher order tangent bundle. Lifting the fluid velocity field to the bundle leads naturally to a semidirect product Lie–Poisson bracket for the conservative dynamics. The elastic stress exerted by the multibead chains on the fluid then follows directly from the same Hamiltonian functional that governs the internal dissipative mechanics of the multibead chains. For chains with three or more beads, the possible bending of the chain introduces an angular momentum flux that is absent for chains with two beads. This flux appears as an asymmetric elastic stress whose antisymmetric part is the divergence of a rank-3 tensor, as in the Cosserats’ theory of couple stresses in media with no internal angular momentum density. We investigate the possibility of an exact closure, passing from a distribution function description to a closed internal state variable description of the fluid suspension, and obtain some sufficient conditions for their existence. The resulting exactly closable models are generalisations of the upper-convected Maxwell model to Hookean bead-spring chains instead of Hookean bead-spring pairs.

Keywords: viscoelastic fluids, kinetic description, higher order tangent bundles, semidirect product Lie–Poisson brackets

1 Introduction

A common microscopic model for a non-Newtonian fluid, e.g. a viscoelastic polymer solution, is that of a *fluid suspension*, which consists of small bodies with internal structure suspended in a Newtonian fluid. The evolution of these small bodies can be described by a *hydrodynamic* part, where the small bodies are advected like Lagrangian markers, and a *dissipative* part, which describes the internal relaxation of the small bodies as well as diffusive effects due to stochastic Brownian forces. The exact configurations of the small bodies are difficult to measure directly and uninteresting for macroscopic experiments, so one often resorts to a probabilistic, or ensemble, description of the small bodies, using an ensemble *distribution function* $\psi(x, y)$ to encode the number density of bodies at position x and with internal configuration y . The stress exerted on the fluid by the suspended bodies is a macroscopic quantity i.e. a function of position only, so it can often be given in terms of some statistical properties of the internal degrees of freedom in the ensemble, for instance certain y -integrals (or y -moments) of the distribution function $\psi(x, y)$.

A familiar example is a dilute suspension of Hookean bead-spring pairs, which is a microscopic realisation of a viscoelastic fluid described by the upper-convected Maxwell model [3, 28]. The internal configuration y is a vector describing the relative displacement of the two beads. The evolution equation for the distribution function $\psi(x, y)$ is a *Liouville equation*, or a *Fokker–Planck equation*, which contains three types of terms, each describing respectively the advection of the beads as Lagrangian markers, the relative motion of the beads to the background flow due to the force of the spring, and diffusion due to stochastic Brownian forces exerted by the suspending fluid. For a Hookean spring, the particle-contributed stress depends solely on the *number density* $n(x) = \int d^n y \psi(x, y)$ and the *conformation tensor* $C^{jk}(x) = \int d^n y y^j y^k \psi(x, y)$, which are the zeroth and second y -moments of ψ respectively. Moreover, these moments of ψ form a *closed system* – the time evolution of $n(x)$ and $C^{jk}(x)$ do not depend on any other y -moments of ψ . The reduced system of equations obtained this way is precisely the upper-convected Maxwell model for the elastic stress.

The above observations can be recast into more abstract geometrical language. The fluid velocity field can be thought of as a vector field \mathbf{u} on a manifold M , while the configuration space for each of the suspended bodies can be thought of as a *fibre bundle* $E \rightarrow M$, which is a smoothly varying assignment of a standard fibre F to each point x in M , written as $F \mapsto F_x$. The standard fibre F is the internal configuration space of a reference copy of the small body, whereas the total space E is the full configuration space of the body in the fluid domain. Certain fibre bundles E admit lifts of a vector field \mathbf{u} on the base manifold M to a vector field $\mathbf{u}^\#$ on E , such that the lift is a *Lie algebra homomorphism*. The flow of the lifted vector field corresponds to the flow of Lagrangian markers in a suitable configuration space. For example, if $E = TM$ is the *tangent bundle*, then the *complete lift* (or *tangent lift*) of vector fields describe the motion of a line element (or a tangent vector) that is frozen into a fluid – the basepoint of the line element moves with the fluid, while the displacement across the line element is stretched by the local velocity gradient. If the evolution of the small bodies can be described purely as Lagrangian markers, then the resulting coupled dynamical system for the fluid and the distribution function ψ can be formulated as a *noncanonical Hamiltonian system*, whose dynamics is completely described by an (abstract) *Poisson bracket* $\{\cdot, \cdot\}$ and a *Hamiltonian functional* H . The system is called noncanonical, because the Poisson bracket $\{\cdot, \cdot\}$ is an abstract, coordinate-free generalisation of the usual Poisson bracket given in canonical coordinates. The Poisson brackets that we will consider belong to the family of *semidirect product Lie–Poisson brackets* [20, 21]. One of the main advantages for such a formulation is that, given an arbitrary Hamiltonian functional for the suspended small bodies, the body force (and hence the stress) exerted on the fluid by the bodies can be calculated from a straightforward manipulation of the Poisson bracket [2, 13]. Semidirect product Lie–Poisson structures have been used to describe ideal fluids [26, 30], complex fluids [1, 2, 9, 12, 13, 19] and magnetohydrodynamics [20, 27].

The dissipative part of the dynamical system, which typically consists of the relaxation of the internal degrees of freedom e.g. motions of the body caused by internal elastic forces, as well as Brownian diffusive effects, can be modelled by a symmetric *dissipation bracket* [1, 2, 9, 25]. This can be thought of as an implementation of the *mobility relations* in Stokes flow that convert any extra forces to a velocity difference with the background flow [2, 12]. Such internal interactions typically do not couple to the macroscopic fluid flow, so the procedure of calculating the stress using the Poisson bracket is still valid. This gives a complete description of the fluid suspension in terms of the usual fluid variables and the distribution function ψ . It is also possible to account for the Newtonian viscous stress of the fluid using dissipation brackets [2, 10, 24]. For the case of a Hookean bead-spring pair suspension, the inclusion of the Newtonian viscous stress leads to the Oldroyd-B model, a generalisation of the upper-convected Maxwell model with nonzero fluid viscosity.

However, the distribution function $\psi(x, y)$ depends on both the internal and macroscopic degrees of freedom, and the evolution equation of $\psi(x, y)$ is a partial differential equation in $\dim(E) + 1$ dimensions (including time), which is much more computationally expensive to solve than a system of partial differential equations in $\dim(M) + 1$ dimensions. For example, for a bead-spring pair suspension in a 3-dimensional domain, the evolution equation for the distribution function is a $6 + 1$ -dimensional partial differential equation. Fortunately, it is not necessary to solve for the full distribution function $\psi(x, y)$ for some cases – it is possible that there exist a finite number of y -integrals (more abstractly, integrals over the fibres F_x) of the distribution function $\psi(x, y)$ that describe the stress tensor fully while forming a closed system of evolution equations. This property is called *finite and exact closure*. When this is possible, it is sufficient to evolve said y -integrals of $\psi(x, y)$, which are x -dependent fields, without having to solve for the full distribution function $\psi(x, y)$. In abstract terms, these y -integrals of $\psi(x, y)$ are geometric objects living on M (sections of some naturally constructed fibre bundles), e.g. tensor fields. This is indeed the case for the Hookean bead-spring pair, for which there exists a closed system of evolution equations for the macroscopic number density $n(x)$ and the conformation tensor $C^{jk}(x)$. Together they are sufficient to describe the particle-contributed stress.

While the upper-convected Maxwell model and its connection with a suspension of bead-spring pairs is well known [3, 28], a straightforward extension of the strategy above produces models for multibead-chain suspensions, namely by looking at fibre bundles known as *higher order tangent bundles* [34]. Loosely speaking, a point in the N^{th} order tangent bundle $T^{(N)}M$ can be thought of as a local $(N + 1)$ -point approximation to a path attached to M . This is a generalisation of the tangent bundle TM , which is the configuration space for tangent vectors, or material line elements. Such fibre bundles admit analogues of the complete lift of vector fields to tangent bundles, also called the *complete lift*. The hydrodynamic part of the evolution of multibead-chains as Lagrangian markers can then be analogously captured by a semidirect product Lie–Poisson bracket. If we choose a dissipation bracket corresponding to a linear mobility relation to describe the response to non-hydrodynamic forces on the multibead-chains, and choose a quadratic energy function analogous to that of Hookean bead-spring pairs, we can show that the resulting system is *closed* – there exists a finite set of moments whose evolution equations do not depend on moments outside of the set, and are also sufficient to describe the stress tensor. These models can be considered as generalisations of the upper-convected Maxwell model from bead-spring pairs to bead-spring chains.

A crucial difference between a multibead-chain with 3 or more beads and a bead-spring pair is that the former can exchange *angular momentum* between fluid parcels i.e. the particle-contributed stress tensor is asymmetric.

This can be understood as follows: a multibead-chain with 3 or more beads is sensitive to the *second derivative* of the background fluid velocity, which means it can detect *vorticity gradients* across fluid parcels. The multibead-chain can *bend*, in the sense that the middle beads are not necessarily aligned with the end-to-end displacement of the chain. This is an effect that is not captured by a bead-spring pair, since it is only sensitive to the local velocity gradient. We will show that for reasonable choices of the internal energy, the antisymmetric part of the stress tensor can be written as the divergence of a 3-index tensor, which we can think of as an *angular momentum flux* across material surfaces. This is consistent with the picture that the suspended multibead-chains have no inertia, and hence have zero internal angular momentum. Thus we have a family of microscopic models for an asymmetric non-Newtonian stress, which supports an angular momentum flux due to internal structure. These are microscopic realisations of the generalised continuum systems considered in [4, 5, 29] that support asymmetric stress tensors. In these continuum systems, the interactions of the internal degrees of freedom can transmit an angular momentum flux, called the *couple stress*. The internal angular momentum density of the multibead-chain suspension is identically zero everywhere, so the instantaneous torque balance is maintained by the divergence of a couple stress. By contrast, in continuum models for suspensions with internal “spin” degrees of freedom such as ferrofluids, couple stresses alone cannot balance the asymmetric hydrodynamic stress, so the internal angular momentum density must evolve dynamically [29, 31].

The outline of the paper is as follows. In section 2 we give an overview of the general mathematical strategy on forming semidirect product Lie–Poisson systems relevant to fluid suspensions, and in section 3 we will apply the strategy to recover the upper-convected Maxwell model for bead-spring pairs, which will serve as a benchmark for the double bracket systems considered later. In section 4 we will consider higher order tangent bundles, and the resulting semidirect product Lie–Poisson bracket obtained from such a construction. As an illustration, we will work out the case for the 3-bead chain in section 5, and examine its similarities and differences with the bead-spring pair in detail. Finally, we will investigate the closure and conservation properties of the general multibead-chain model in section 6, by working out the explicit form of the Poisson bracket.

2 Mathematical preliminaries

This section reviews some of the geometrical machinery used in constructing Poisson brackets relevant for the dynamics of fluid suspensions, so that we can formulate the conservative part of the dynamics as a *noncanonical Hamiltonian system* [17, 20, 21, 22, 23, 26]. Most technical hypotheses will be suppressed. In particular, various smoothness and decay assumptions on infinite-dimensional spaces will be implicit. We assume all manifolds to be oriented for simplicity - the following arguments work on non-orientable manifolds if we replace every instant of “top-degree differential form” or “volume form” with “density”.

A complementary approach formulates the conservative part of the suspension dynamics in terms of a *variational principle*. We will not pursue this approach in this paper. References with an emphasis on fluid dynamics can be found in [11, 14, 15, 22, 30].

2.1 Lie algebras

An *abstract Lie algebra* \mathfrak{g} is a vector space together with a bilinear \mathfrak{g} -valued map $[\cdot, \cdot] : \mathfrak{g} \times \mathfrak{g} \rightarrow \mathfrak{g}$ called the *Lie bracket*, such that, for all $u, v, w \in \mathfrak{g}$:

$$[u, v] = -[v, u], \quad (\text{antisymmetry}) \quad (2.1)$$

$$[[u, v], w] + [[v, w], u] + [[w, u], v] = 0. \quad (\text{Jacobi identity}) \quad (2.2)$$

The primary example relevant to fluid dynamics is the *Lie algebra of vector fields* on a manifold M , denoted $\text{Vect}(M)$. In tensor calculus and differential geometry, vector fields \mathbf{u} are associated with first order differential operators $u^i \partial / \partial x^i$ corresponding to the *directional derivative* of a function on M along \mathbf{u} . This is sometimes written as $\mathbf{u} \cdot \nabla$.

The Lie bracket on $\text{Vect}(M)$ the commutator of first order differential operators:

$$[u, v]^i \frac{\partial f}{\partial x^i} := u^j \frac{\partial}{\partial x^j} \left(v^i \frac{\partial f}{\partial x^i} \right) - v^j \frac{\partial}{\partial x^j} \left(u^i \frac{\partial f}{\partial x^i} \right) = \left(u^j \frac{\partial v^i}{\partial x^j} - v^j \frac{\partial u^i}{\partial x^j} \right) \frac{\partial f}{\partial x^i}. \quad (2.3)$$

2.2 Noncanonical Hamiltonian mechanics

Many conservative physical systems can be formulated in terms of noncanonical Hamiltonian systems. Detailed mathematical expositions can be found in [17, 21, 23]. The review articles [26, 30, 35] cover noncanonical Hamiltonian mechanics with an emphasis on fluid dynamics.

2.2.1 Functional derivatives

Let V be a Banach or Frechét space, not necessarily finite dimensional. Let V^* be its *smooth dual*, which means that it is subspace of the full continuous dual of V that has a weakly non-degenerate pairing with V . If $F : V \rightarrow \mathbb{R}$ is a functional on V , then its *functional derivative* at $v \in V$ is an element $\delta F/\delta v \in V^*$, such that

$$\left\langle \frac{\delta F}{\delta v}[v], w \right\rangle = \lim_{\epsilon \rightarrow 0} \frac{F[v + \epsilon w] - F[v]}{\epsilon}, \quad (2.4)$$

where $\langle \cdot, \cdot \rangle$ is the dual pairing between V and V^* . We implicitly assume that the functionals we are working with are sufficiently regular, so that (2.4) makes sense and $\delta F/\delta v$ lies in an appropriate smooth dual space V^* .

For example, if $C^\infty(\mathbb{R}^n)$ is the space of smooth functions on \mathbb{R}^n , then its smooth dual space can be taken to be the space of smooth n -forms $\Omega^n(\mathbb{R}^n)$, with typical element $\alpha d^n x$, and the pairing between $f \in C^\infty(\mathbb{R}^n)$ and $\alpha d^n x \in \Omega^n(\mathbb{R}^n)$ is by integration:

$$\langle \alpha d^n x, f \rangle = \int d^n x \alpha f. \quad (2.5)$$

Here and henceforth decay conditions at infinity will be implicitly assumed. If $F[f] = \int d^n x \varphi(f, \partial f/\partial x^i)$, then integrating by parts and assuming boundary terms vanish gives

$$\frac{\delta F}{\delta f} = \left(\frac{\partial \varphi}{\partial f} - \frac{\partial}{\partial x^i} \frac{\partial \varphi}{\partial (\frac{\partial f}{\partial x^i})} \right) d^n x, \quad (2.6)$$

which is the usual Euler–Lagrange variational derivative of functionals. The factor $d^n x$ is usually suppressed. This reflects a choice of a standard volume element $d^n x$ in \mathbb{R}^n .

2.2.2 Poisson brackets

Consider the space of sufficiently regular functionals $\mathcal{F}(V)$ on a vector space V . An (abstract) *Poisson bracket* is a bilinear operation on functionals, $\{\cdot, \cdot\} : \mathcal{F}(V) \times \mathcal{F}(V) \rightarrow \mathcal{F}(V)$, such that for all $F, G, H \in \mathcal{F}(V)$:

$$\{F, G\} = -\{G, F\}, \quad (\text{antisymmetry}) \quad (2.7)$$

$$\{F, GH\} = \{F, G\}H + \{F, H\}G, \quad (\text{Leibniz/product rule}) \quad (2.8)$$

$$0 = \{\{F, G\}, H\} + \{\{G, H\}, F\} + \{\{H, F\}, G\}, \quad (\text{Jacobi identity}) \quad (2.9)$$

whenever the expressions are well-defined. The resemblance with Lie algebra is more than superficial – there is a crucial Poisson bracket that can be constructed from a Lie algebra, called the *Lie–Poisson bracket*, which we will make use of extensively.

A *noncanonical Hamiltonian system* on V is a dynamical system where the time evolution of functionals $F[v]$ is given in terms of a Poisson bracket $\{\cdot, \cdot\}$ and a chosen Hamiltonian functional $H[v]$:

$$\dot{F}[v] = \{F, H\}[v]. \quad (2.10)$$

This is a generalisation of usual Hamiltonian mechanics on the classical phase space \mathbb{R}^{2n} . We obtain the evolution equation for $w \in V$ using the functional chain rule:

$$\left\langle \frac{\delta F}{\delta v}[w], \dot{w} \right\rangle = \dot{F}[w] = \{F, H\}[w] = \left\langle \frac{\delta F}{\delta v}[w], J[w] \left(\frac{\delta H}{\delta v}[w] \right) \right\rangle. \quad (2.11)$$

If V is infinite-dimensional, the evolution equation for w is recovered in a weak sense. The bracket is formally guaranteed to be bilinear on $\delta F/\delta v, \delta H/\delta v$ by (2.8), so we can always write $\{F, H\}$ in the form shown in the rightmost expression in (2.11). The linear operator $J[w] : V^* \rightarrow V$ called the *Poisson tensor*. In contrast to Hamiltonian mechanics on \mathbb{R}^{2n} in canonical coordinates, the Poisson tensor can vary with w in general. Moreover, there can be non-constant functionals $C[v]$ such that $\{F, C\} = 0$ for arbitrary functionals F in this formalism. Any such C is called a *Casimir functional*. The local theory of noncanonical Poisson brackets in finite dimensions is extensively studied in [33].

2.3 Lie–Poisson dynamics on the dual of a Lie algebra

The Jacobi identity for Poisson brackets on functionals is typically difficult and unenlightening to verify from direct computation. In this section we describe the *Lie–Poisson bracket* associated to a Lie algebra \mathfrak{g} , which is a

noncanonical Poisson bracket for functionals on the dual \mathfrak{g}^* of \mathfrak{g} . This provides a wide class of Poisson brackets that automatically satisfy the Jacobi identity.

Given a Lie algebra \mathfrak{g} , consider the smooth dual \mathfrak{g}^* of \mathfrak{g} , with the dual pairing written as $\langle \cdot, \cdot \rangle$. For example, if $\mathfrak{g} = \text{Vect}(M)$ is the Lie algebra of vector fields u^i on a manifold M , the dual space will consist of elements of the form $m_i d^n x$, where the dual pairing is given by integration $\langle m_i d^n x, u^i \rangle = \int d^n x m_i u^i$. The elements $m_i d^n x$ can be thought of as the momentum density of a fluid when u^i is the vector field generating the flow of a fluid. The factor $d^n x$ is usually suppressed from the notation.

The space of sufficiently regular functionals $\mathcal{F}(\mathfrak{g}^*)$ on the dual \mathfrak{g}^* of the Lie algebra \mathfrak{g} is automatically equipped with a Poisson bracket, called the (\pm) -Lie-Poisson bracket:

$$\{F, G\}_{LP, \pm}[\mathbf{m}] := \pm \left\langle \mathbf{m}, \left[\frac{\delta F}{\delta \mathbf{m}}[\mathbf{m}], \frac{\delta G}{\delta \mathbf{m}}[\mathbf{m}] \right] \right\rangle, \quad (2.12)$$

where $[\cdot, \cdot]$ is the Lie bracket on \mathfrak{g} . In general $\delta F / \delta \mathbf{m}$ is an element in \mathfrak{g}^{**} , but we will only work with sufficiently regular F , such that $\delta F / \delta \mathbf{m}$ lies in the image of the natural embedding $\mathfrak{g} \hookrightarrow \mathfrak{g}^{**}$. When this condition is met, the Lie brackets of such functional derivatives are well-defined. The fact that $\{\cdot, \cdot\}_{LP, \pm}$ is a Poisson bracket follows from $[\cdot, \cdot]$ being a Lie bracket. The proof can be found in [21, 22, 23].

2.4 Semidirect product Lie algebras

Since any Lie algebra \mathfrak{g} automatically induces a Lie-Poisson bracket for functionals on its dual $\mathcal{F}(\mathfrak{g}^*)$, a strategy to enlarge the Lie algebra \mathfrak{g} allows us to obtain new but related Lie-Poisson brackets from old ones. One popular strategy to enlarge Lie algebras is to form *semidirect products*, which involves finding *representations* of the Lie algebra. We will use this later to construct Lie-Poisson systems that describe some dilute suspensions in fluids with internal degrees of freedom. The Poisson bracket for ideal compressible hydrodynamics is also constructed this way.

Let \mathfrak{g} be a Lie algebra, V a vector space, and let $\text{End}(V)$ denote the space of linear maps on V . A *representation* of \mathfrak{g} on V is an assignment $\phi : \mathfrak{g} \rightarrow \text{End}(V)$, such that, for all $X, Y \in \mathfrak{g}$ and all $v \in V$,

$$\phi(X + Y) \cdot v = \phi(X) \cdot v + \phi(Y) \cdot v, \quad (\text{linearity}) \quad (2.13)$$

$$\phi([X, Y]) \cdot v = [\phi(X), \phi(Y)] \cdot v, \quad (\text{homomorphism property}) \quad (2.14)$$

where $[\phi(X), \phi(Y)] = \phi(X)\phi(Y) - \phi(Y)\phi(X)$ is the operator commutator of linear maps on V . The main example is the representation of the Lie algebra of vector fields on smooth functions, given by

$$\phi(\mathbf{u}) \cdot f = u^i \frac{\partial f}{\partial x^i}, \quad \text{for } \mathbf{u} \in \text{Vect}(M) \text{ and } f \in C^\infty(M). \quad (2.15)$$

The symbol ϕ is sometimes suppressed when the context is clear. In our notation, $\mathbf{u} \cdot f$ denotes the action of the vector field \mathbf{u} on the function f by differentiation. This is more commonly written as $\mathbf{u} \cdot \nabla f$, but we will avoid the more common notation because we need vector fields to act on other objects in less obvious ways later.

Given a Lie algebra \mathfrak{g} and a representation ϕ of \mathfrak{g} on a vector space V , we can form the *semidirect product Lie algebra* $\mathfrak{g}_s = \mathfrak{g} \ltimes V$. The semidirect product $\mathfrak{g} \ltimes V$ is the direct sum $\mathfrak{g} \oplus V$ as a vector space, so a general element of $\mathfrak{g} \ltimes V$ is (X, v) for $X \in \mathfrak{g}, v \in V$. The Lie bracket on $\mathfrak{g} \ltimes V$ is defined as

$$[(X, v), (Y, w)] := ([X, Y], \phi(X) \cdot w - \phi(Y) \cdot v), \quad \text{for } (X, v), (Y, w) \in \mathfrak{g} \ltimes V. \quad (2.16)$$

For example, in the semidirect product Lie algebra $\text{Vect}(M) \ltimes C^\infty(M)$, the Lie bracket is given by

$$[(u^i, f), (v^i, g)] = ([u, v]^i, u^i \frac{\partial g}{\partial x^i} - v^i \frac{\partial f}{\partial x^i}), \quad (2.17)$$

for $\mathbf{u}, \mathbf{v} \in \text{Vect}(M)$ and $f, g \in C^\infty(M)$.

If we consider a Lie algebra \mathfrak{g} and multiple representations $\phi_a : \mathfrak{g} \rightarrow \text{End}(V_a)$ of \mathfrak{g} on V_a ($a = 1, \dots, N$), then the semidirect product Lie algebra with all such representations $\mathfrak{g} \ltimes (V_1 \oplus \dots \oplus V_N)$ is $\mathfrak{g} \oplus V_1 \oplus \dots \oplus V_N$ as a vector space, with the following Lie bracket:

$$[(X, v_1, \dots, v_N), (Y, w_1, \dots, w_N)] = ([X, Y], \phi_1(X) \cdot w_1 - \phi_1(Y) \cdot v_1, \dots, \phi_N(X) \cdot w_N - \phi_N(Y) \cdot v_N), \quad (2.18)$$

for $X, Y \in \mathfrak{g}$ and $v_a, w_a \in V_a$.

2.5 The Lie–Poisson bracket on the dual of a semidirect product Lie algebra

Let $\mathfrak{g}_s = \mathfrak{g} \ltimes (V_1 \oplus \dots \oplus V_N)$ be a semidirect product Lie algebra, with notation as above. The dual space \mathfrak{g}_s^* of \mathfrak{g}_s is isomorphic to $\mathfrak{g}_s^* = \mathfrak{g}^* \oplus V_1^* \oplus \dots \oplus V_N^*$ as a vector space. The Lie–Poisson bracket for functionals $\mathcal{F}(\mathfrak{g}_s^*)$ can be written as, for $\mathbf{m} \in \mathfrak{g}^*$ and $\mu_a \in V_a^*$ for $a = 1, \dots, N$:

$$\begin{aligned} \{F, G\}_{LP, \pm}[\mathbf{m}, \mu_1, \dots, \mu_N] &= \pm \left\langle (\mathbf{m}, \mu_1, \dots, \mu_N), \left[\left(\frac{\delta F}{\delta \mathbf{m}}, \frac{\delta F}{\delta \mu_1}, \dots, \frac{\delta F}{\delta \mu_N} \right), \left(\frac{\delta G}{\delta \mathbf{m}}, \frac{\delta G}{\delta \mu_1}, \dots, \frac{\delta G}{\delta \mu_N} \right) \right] \right\rangle, \\ &= \pm \left(\left\langle \mathbf{m}, \left[\frac{\delta F}{\delta \mathbf{m}}, \frac{\delta G}{\delta \mathbf{m}} \right] \right\rangle + \sum_{a=1}^N \left\langle \mu_a, \phi_a \left(\frac{\delta F}{\delta \mathbf{m}} \right) \cdot \frac{\delta G}{\delta \mu_a} - \phi_a \left(\frac{\delta G}{\delta \mathbf{m}} \right) \cdot \frac{\delta F}{\delta \mu_a} \right\rangle \right). \end{aligned} \quad (2.19)$$

Suppose that one has a Hamiltonian functional $H = H[\mathbf{m}, \mu_1, \dots, \mu_N]$. The noncanonical Lie–Poisson dynamics given by this Hamiltonian is $\dot{F} = \{F, H\}$. In particular:

$$\begin{aligned} &\left\langle \frac{\delta F}{\delta \mathbf{m}}, \dot{\mathbf{m}} \right\rangle + \sum_{a=1}^N \left\langle \frac{\delta F}{\delta \mu_a}, \dot{\mu}_a \right\rangle \\ &= \pm \left(\left\langle \mathbf{m}, \left[\frac{\delta F}{\delta \mathbf{m}}, \frac{\delta H}{\delta \mathbf{m}} \right] \right\rangle + \sum_{a=1}^N \left\langle \mu_a, \phi_a \left(\frac{\delta F}{\delta \mathbf{m}} \right) \cdot \frac{\delta H}{\delta \mu_a} \right\rangle - \sum_{a=1}^N \left\langle \mu_a, \phi_a \left(\frac{\delta H}{\delta \mathbf{m}} \right) \cdot \frac{\delta F}{\delta \mu_a} \right\rangle \right). \end{aligned} \quad (2.20)$$

Since F is arbitrary, we can take $F = F[\mu_b]$ only for some $b = 1, \dots, N$. This gives

$$\left\langle \frac{\delta F}{\delta \mu_b}, \dot{\mu}_b \right\rangle = \mp \left\langle \mu_b, \phi_b \left(\frac{\delta H}{\delta \mathbf{m}} \right) \cdot \frac{\delta F}{\delta \mu_b} \right\rangle = \mp \left\langle \phi_b \left(\frac{\delta H}{\delta \mathbf{m}} \right)^\dagger \cdot \mu_b, \frac{\delta F}{\delta \mu_b} \right\rangle, \quad (2.21)$$

where $\phi_b(\delta H/\delta \mathbf{m})^\dagger : V_b^* \rightarrow V_b^*$ is the formal adjoint to $\phi_b(\delta H/\delta \mathbf{m}) : V_b \rightarrow V_b$. For applications relevant to fluid dynamics, “taking the adjoint” usually means integrating by parts, assuming boundary terms vanish. The time evolution of μ_b is then

$$\dot{\mu}_b = \mp \phi_b \left(\frac{\delta H}{\delta \mathbf{m}} \right)^\dagger \cdot \mu_b. \quad (2.22)$$

In fluid dynamics, the relevant Lie algebra is $\text{Vect}(M)$, and $\delta H/\delta \mathbf{m} = \mathbf{u}$ is usually the fluid velocity, so we can think of (2.22) as corresponding to μ_b being “materially advected” by the fluid velocity field as Lagrangian markers attached to fluid parcels. Thus the dual spaces to the representations of $\text{Vect}(M)$ correspond to “advected degrees of freedom”. This has been used to construct, for example, the ideal compressible magnetohydrodynamics (MHD) equations, in which the magnetic field is “frozen” into the fluid [20, 27].

3 The bead-spring pair equations

In this section we formulate the bead-spring pair equations as a noncanonical Hamiltonian system. The Lie–Poisson bracket we construct coincides with the one in [12]. The double bracket formulation is also considered in order to incorporate dissipative and diffusive effects. We recover the kinetic equation for bead-spring pairs in [3, 28] with this formulation.

3.1 Tangent bundles

The configuration space of small bead-spring pairs is most naturally described as a tangent bundle. We briefly recall the notion of a tangent bundle and explain why this is the case.

Let M be an n -dimensional manifold (it is sufficient to take $M = \mathbb{R}^n$ for the applications later). Consider the space of *smooth paths* on M , i.e. the collection of smooth maps $\alpha : I \rightarrow M$, where I is a (fixed) closed interval in \mathbb{R} containing 0 in its interior. This space is infinite-dimensional, but we can take certain quotients to obtain finite-dimensional approximations.

Consider the equivalence class of paths under the equivalence relation $\overset{(1)}{\sim}$, given by

$$\alpha \overset{(1)}{\sim} \beta \text{ if and only if } \alpha(0) = \beta(0), \text{ and } \alpha'(0) = \beta'(0). \quad (3.1)$$

If α^i and β^i are the coordinates for the paths α, β respectively, then the equivalence relation is given by $2n$ equations:

$$\alpha^i(0) = \beta^i(0), \quad \frac{d\alpha^i}{dt}(0) = \frac{d\beta^i}{dt}(0). \quad (3.2)$$

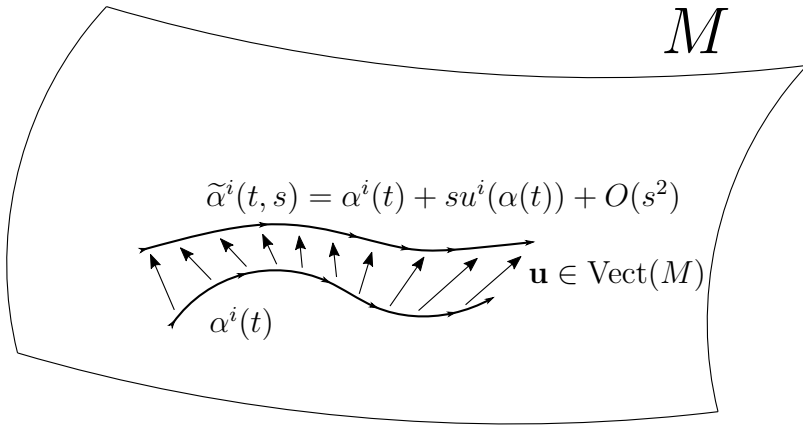


Figure 1: The effect of the flow of $\mathbf{u} \in \text{Vect}(M)$ on the path $\alpha^i(t)$.

This equivalence relation is coordinate independent. We denote each equivalence class by (x^i, y^i) , where x^i is the coordinates of $\alpha(0)$ and y^i the coordinates of $d\alpha/dt(0)$, where $\alpha(t)$ is a representing element of the equivalence class. Each of these equivalence classes is nonempty because we can construct a local path $\alpha^i(t) = x^i + y^i t + O(t^2)$. The space of all such equivalence classes is called the *tangent bundle* TM of M , and is a $2n$ -dimensional manifold.

A general point on the tangent bundle TM can be thought of as a point x^i on M , together with a tangent vector y^i attached to the point $x^i \in M$. Informally, this is like a two-point approximation to a small segment of a curve in M . This physical picture of a tangent bundle suggests that TM is indeed the correct configuration space of small bead-spring pairs living on M .

3.2 Complete/Tangent lift of vector fields on M to TM

Since TM is constructed naturally from M , we expect vector fields $\mathbf{u} \in \text{Vect}(M)$ on M to act on geometrical objects living on TM (functions, tensors, etc.) in a nice way. This allow us to construct a semidirect product $\text{Vect}(M) \ltimes C^\infty(TM)$ of vector fields on M acting on functions on TM .

The smooth dual space to $C^\infty(TM)$ can be taken as $\Omega^{2n}(TM)$, the space of volume forms on TM . A typical element of $\Omega^{2n}(TM)$ is a $2n$ -form $\psi(x, y) d^n x d^n y$, with integration on TM being the dual pairing with $C^\infty(TM)$. It has a natural interpretation as a *distribution function* of bead-spring pairs in configuration space. This semidirect product formulation describes the dynamics of the bead-spring pairs as Lagrangian markers embedded in the fluid.

The vector field $\mathbf{u} \in \text{Vect}(M)$ induces a vector field $\mathbf{u}^\# \in \text{Vect}(TM)$, called the *complete lift* or *tangent lift* [34], which is described as follows. Consider the effect of the flow of u^i on a path $\alpha^i(t)$ on M . For some small flow parameter s , the path $\alpha^i(t)$ is deformed by the flow, as in figure 1):

$$\tilde{\alpha}^i(t, s) = \alpha^i(t) + s u^i(\alpha(t)) + O(s^2) \quad (3.3)$$

Now consider how the $\stackrel{(1)}{\sim}$ -equivalence class of $\tilde{\alpha}^i(t, s)$, i.e. its value at $t = 0$ and its first t -derivative at $t = 0$, changes with s . Let

$$\tilde{x}^i(s) = \tilde{\alpha}^i(0, s), \quad x^i = \tilde{x}^i(0), \quad (3.4)$$

$$\tilde{y}^i(s) = \frac{\partial \tilde{\alpha}^i}{\partial t}(0, s), \quad y^i = \tilde{y}^i(0). \quad (3.5)$$

Then

$$\tilde{x}^i(s) = \alpha^i(0) + s u^i(\alpha(0)) + O(s^2) = x^i + s u^i(x) + O(s^2), \quad (3.6)$$

$$\tilde{y}^i(s) = \frac{d\alpha^i}{dt}(0) + s \frac{\partial u^i}{\partial x^j}(\alpha(0)) \frac{d\alpha^j}{dt}(0) + O(s^2) = y^i + s \frac{\partial u^i}{\partial x^j}(x) y^j + O(s^2). \quad (3.7)$$

By taking the order s terms in the above equations, we obtain the complete lift of a vector field \mathbf{u} on M to a vector field $\mathbf{u}^\#$ on the tangent bundle TM . The components of $\mathbf{u}^\#$ with respect to the coordinate system (x^i, y^i) are

$$\left(u^i(x), \frac{\partial u^i}{\partial x^j}(x) y^j \right). \quad (3.8)$$

The associated differential operator for $\mathbf{u}^\# \in \text{Vect}(TM)$ that acts on smooth functions on TM is

$$u^i(x) \frac{\partial}{\partial x^i} + \frac{\partial u^i}{\partial x^j}(x) y^j \frac{\partial}{\partial y^i}. \quad (3.9)$$

The complete lift $\mathbf{u} \mapsto \mathbf{u}^\#$ is a *Lie algebra homomorphism* $\text{Vect}(M) \rightarrow \text{Vect}(TM)$ with respect to the commutator bracket of vector fields on M and TM respectively:

$$([\mathbf{u}, \mathbf{v}]_M)^\# = [\mathbf{u}^\#, \mathbf{v}^\#]_{TM}, \quad (3.10)$$

where the subscripts indicate the spaces on which the vector fields live. A proof sketch can be found in appendix A. Vector fields $\mathbf{u} \in \text{Vect}(M)$ on M can thus act on functions $f \in C^\infty(TM)$ on TM via $f \mapsto \mathbf{u}^\# \cdot f$, and moreover this action is a Lie algebra representation:

$$[\mathbf{u}^\#, \mathbf{v}^\#]_{TM} \cdot f = \mathbf{u}^\# \cdot \mathbf{v}^\# \cdot f - \mathbf{v}^\# \cdot \mathbf{u}^\# \cdot f = ([\mathbf{u}, \mathbf{v}]_M)^\# \cdot f. \quad (3.11)$$

So we can add this representation of $\text{Vect}(M)$ on $C^\infty(TM)$ to the semidirect product $\text{Vect}(M) \ltimes C^\infty(M)$ relevant to ideal compressible fluid dynamics to obtain the Lie algebra

$$\mathfrak{g}_s = \text{Vect}(M) \ltimes (C^\infty(M) \oplus C^\infty(TM)), \quad (3.12)$$

which will be relevant to describing suspensions of bead-spring pairs in compressible fluids.

3.3 The ψ -subbracket for the distribution function of bead-spring pairs

Now we take the dual \mathfrak{g}_s^* of $\mathfrak{g}_s = \text{Vect}(M) \ltimes (C^\infty(M) \oplus C^\infty(TM))$ and consider the Lie–Poisson dynamics for functionals on \mathfrak{g}_s^* . As a vector space, \mathfrak{g}_s^* consists of elements of the form (m_i, ρ, ψ) , where $m_i d^n x$ is the momentum density of the fluid, $\rho d^n x$ is the mass density of the fluid, and $\psi(x, y) d^n x d^n y$ can be interpreted as the number density of bead-spring pairs with centre located at x^i and relative displacement y^i between the beads. The dual pairing between $C^\infty(TM)$ and $\Omega^{2n}(TM)$ is given by integration over TM i.e. over all x, y .

The minus Lie–Poisson bracket for functionals $F[\mathbf{m}, \rho, \psi], G[\mathbf{m}, \rho, \psi]$ is

$$\begin{aligned} \{F, G\}[\mathbf{m}, \rho, \psi] &= - \left\langle \mathbf{m}, \left[\frac{\delta F}{\delta \mathbf{m}}, \frac{\delta G}{\delta \mathbf{m}} \right] \right\rangle - \left\langle \rho, \frac{\delta F}{\delta \mathbf{m}} \cdot \frac{\delta G}{\delta \rho} - \frac{\delta G}{\delta \mathbf{m}} \cdot \frac{\delta F}{\delta \rho} \right\rangle - \left\langle \psi, \left(\frac{\delta F}{\delta \mathbf{m}} \right)^\# \cdot \frac{\delta G}{\delta \psi} - \left(\frac{\delta G}{\delta \mathbf{m}} \right)^\# \cdot \frac{\delta F}{\delta \psi} \right\rangle, \\ &= \{F, G\}_{fluids} + \{F, G\}_\psi, \end{aligned} \quad (3.13)$$

where we have separated the usual fluid bracket and the extra terms, which we will call the ψ -subbracket, as follows:

$$\{F, G\}_{fluids} = - \left\langle \mathbf{m}, \left[\frac{\delta F}{\delta \mathbf{m}}, \frac{\delta G}{\delta \mathbf{m}} \right] \right\rangle - \left\langle \rho, \frac{\delta F}{\delta \mathbf{m}} \cdot \frac{\delta G}{\delta \rho} - \frac{\delta G}{\delta \mathbf{m}} \cdot \frac{\delta F}{\delta \rho} \right\rangle, \quad (3.14)$$

$$\{F, G\}_\psi = - \left\langle \psi, \left(\frac{\delta F}{\delta \mathbf{m}} \right)^\# \cdot \frac{\delta G}{\delta \psi} - \left(\frac{\delta G}{\delta \mathbf{m}} \right)^\# \cdot \frac{\delta F}{\delta \psi} \right\rangle. \quad (3.15)$$

Now focus on $M = \mathbb{R}^n$ and consider Hamiltonians of the form

$$H = H_{fluids}[\mathbf{m}, \rho] + H_s[\psi], \quad (3.16)$$

where H_{fluids} is the usual ideal compressible fluid Hamiltonian

$$H = H_{fluids}[\mathbf{m}, \rho] = \int d^n x \left(\frac{m_i m_j \delta^{ij}}{2\rho} + \rho U(\rho) \right), \quad (3.17)$$

and $H_s[\psi]$ is the internal free energy of the bead-spring pairs, which is unspecified for now.

The coordinate expression of the subbracket (3.15) coincides with the ψ -subbracket in [12], obtained from direct inspection. Writing $u^i = \delta H / \delta m_i$, the subbracket $\{F, H\}_\psi$ is

$$\begin{aligned} \{F, H\}_\psi &= - \int d^n x d^n y \psi \left[\frac{\delta F}{\delta m_i} \frac{\partial}{\partial x^i} \left(\frac{\delta H_s}{\delta \psi} \right) + \frac{\partial}{\partial x^j} \left(\frac{\delta F}{\delta m_i} \right) y^j \frac{\partial}{\partial y^i} \left(\frac{\delta H_s}{\delta \psi} \right) \right] \\ &\quad - \int d^n x d^n y \psi \left[-u^i \frac{\partial}{\partial x^i} \left(\frac{\delta F}{\delta \psi} \right) - \frac{\partial u^i}{\partial x^j} y^j \frac{\partial}{\partial y^i} \left(\frac{\delta F}{\delta \psi} \right) \right], \\ &= \left\langle \frac{\delta F}{\delta m_i}, \int d^n y \left[-\psi \frac{\partial}{\partial x^i} \left(\frac{\delta H_s}{\delta \psi} \right) + \frac{\partial}{\partial x^j} \left(\psi y^j \frac{\partial}{\partial y^i} \left(\frac{\delta H_s}{\delta \psi} \right) \right) \right] \right\rangle \\ &\quad + \left\langle \frac{\delta F}{\delta \psi}, -\frac{\partial}{\partial x^i} (u^i \psi) - \frac{\partial}{\partial y^i} \left(\frac{\partial u^i}{\partial x^j} y^j \psi \right) \right\rangle, \end{aligned} \quad (3.18)$$

from which we obtain

$$\dot{\psi} = -\frac{\partial}{\partial x^i} (u^i \psi) - \frac{\partial}{\partial y^i} \left(\frac{\partial u^i}{\partial x^j} y^j \psi \right), \quad (3.19)$$

$$\mathcal{F}_i = \int d^n y \left[-\psi \frac{\partial}{\partial x^i} \left(\frac{\delta H_s}{\delta \psi} \right) + \frac{\partial}{\partial x^j} \left(\psi y^j \frac{\partial}{\partial y^i} \left(\frac{\delta H_s}{\delta \psi} \right) \right) \right], \quad (3.20)$$

where \mathcal{F}_i is the extra force on the fluid due to the suspension.

The Lie–Poisson bracket gives the terms in the “Liouville equation” for the distribution function of bead-spring pairs due to beads advecting with the flow like Lagrangian markers (see [3, 28]). We remark that:

1. If there are no bead-bead interactions and there is no diffusion, the system is Hamiltonian, because the motion of Lagrangian marker particles in a fluid is time-reversible. Since a sufficiently small spherical bead in a Stokes flow is well-approximated by a Lagrangian marker, the “advective” part of the Liouville equation for the distribution function can be captured by the semidirect product Lie–Poisson formulation. However, while the motion of a Lagrangian marker in Stokes flow is time-reversible, the motion of an elastic body, e.g. a Hookean spring, in a Stokes flow is *not* time reversible. We need a *dissipation bracket* to describe the effect of the internal elastic forces within the body.
2. The semidirect product Lie–Poisson formulation implements the following physical principles:
 - Energy is conserved: $\dot{H} = \{H, H\} = 0$.
 - The bead-spring pairs evolve in time as Lagrangian marker particles, in the sense made precise by the construction of $\mathbf{u}^\#$ in section 3.2.

From these two facts, the force of the bead-spring pairs on the fluid can be deduced from the conservation of total energy and Newton’s third law, since we know how the fluid acts on the suspension. This often involves a lot of uninformative manipulations if done directly from the evolution equations. The semidirect product Lie–Poisson formulation provides an expedient way for the force \mathcal{F}_i on the fluid by the suspension to be calculated from the energy $H_s[\psi]$, via direct manipulation of the terms in the subbracket due to ψ . This has been emphasised in [13] and applied in [2] as a uniform way to derive expressions for stress tensors for different semidirect product Lie–Poisson structures.

Since \mathcal{F}_i is a y -integral against ψ , we will find that for reasonable choices of $H_s[\psi]$, the force can be written as the divergence of a stress tensor, and that the stress tensor depends on y -moments of ψ i.e. combinations $\int d^n y p(y) \psi$ for polynomials $p(y)$.

3.4 The dissipation bracket and double bracket dynamics

To extend the noncanonical Hamiltonian formulation to dissipative systems, it is customary to include an additional symmetric positive semidefinite *dissipation bracket* (\cdot, \cdot) , such that

$$\dot{F} = \{F, H\} - \frac{1}{\zeta} (F, H), \quad (3.21)$$

where $1/\zeta > 0$ is the *mobility* parameter. For the bead-chain model, the dissipation bracket is an approximate implementation of the mobility relations in a Stokes flow, which relate the velocity of a bead relative to the fluid around it to any additional forces on the bead.

It is common (although not necessary) to require the bracket to be *bilinear* and satisfy the *Leibniz/product rule*:

$$(FG, H) = F(G, H) + (F, H)G, \quad (3.22)$$

whenever the terms are well-defined. These requirements allows us to write the dissipation bracket of two functionals in a similar manner to (2.11). If F, H are two functionals on the vector space V , the bracket (F, H) can be written as

$$(F, H)[w] = \left\langle \frac{\delta F}{\delta v}, K[w] \left(\frac{\delta H}{\delta v} [w] \right) \right\rangle, \quad (3.23)$$

where w is an arbitrary element in V , and $K[w] : V^* \rightarrow V$ is some formally self-adjoint linear operator that varies with w . By a similar argument used in (2.11), the evolution equation for $w \in V$ can be recovered in a weak sense from (3.21).

There is no obvious geometric justification for the dissipation bracket, unlike the Poisson bracket. The dissipation brackets is mainly motivated by thermodynamic principles, where the double bracket formulation

is used to model non-equilibrium thermodynamics. Discussion on double bracket dynamics can be found in [2, 25]. A recent review in the context of viscoelastic fluids can also be found in [19].

In the non-equilibrium thermodynamics of a *closed system*, energy is conserved while entropy is produced. One often requires that the Hamiltonian functional H to be split into two parts $H = U - \mathcal{S}$, where U is the energy of the system and \mathcal{S} is an entropy-like quantity. The functionals are chosen such that \mathcal{S} is a Casimir functional of the Poisson bracket and U is in the kernel of the dissipation bracket [2, 24, 25]. We will however focus on *isothermal* systems, where the fluid suspension is held at constant temperature by an external thermal bath. This is an *open system*, and in such a system the *free energy* decreases towards a minimum while energy is not necessarily conserved. Thus we interpret the Hamiltonian functional H as a free energy that is non-increasing in time:

$$\dot{H} = -\frac{1}{\zeta}(H, H) \leq 0. \quad (3.24)$$

We now describe a dissipation bracket that gives the correct evolution equation for the distribution function ψ . If $M = \mathbb{R}^n$, then TM can be thought of as \mathbb{R}^{2n} with coordinates (x^i, y^i) . Let δ_{ij} denote the standard metric on \mathbb{R}^n . Then we can introduce a metric on TM given by

$$ds^2 = \delta_{ij}dx^i dx^j + \delta_{ij}dy^i dy^j. \quad (3.25)$$

This is positive definite. The generalisation of this metric to general tangent bundles TM of a Riemannian manifold M is called the *Sasaki metric* as studied in [34]. (See appendix B for more details.) For any $\lambda > 0$

$$ds^2(\lambda) = \delta_{ij}dx^i dx^j + \lambda\delta_{ij}dy^i dy^j, \quad (3.26)$$

is also a valid Riemannian metric on TM . We choose $\lambda = 1/2$ so that the equations we derive later coincide with those in [3, 28]. This is equivalent to rescaling the y -coordinate. The hydrodynamic part of the evolution equation for ψ is invariant under rescaling of the y -coordinate. In rheological applications, it is typical to consider the bead-spring length scale $|y|$ to be much shorter than the flow length scale $|x|$, and we can adjust the factors in the metric as appropriate to reflect this.

To mimic the Lie–Poisson bracket as closely as possible, consider

$$(F, G) = \left\langle \psi, \tilde{g} \left(d \left(\frac{\delta F}{\delta \psi} \right), d \left(\frac{\delta G}{\delta \psi} \right) \right) \right\rangle, \quad (3.27)$$

where \tilde{g} is the inverse of the metric (3.26) with $\lambda = 1/2$ on TM . The coordinate expression for (F, G) is

$$\begin{aligned} (F, G) &= \int d^n x d^n y \, \psi \left[\delta^{ij} \frac{\partial}{\partial x^i} \left(\frac{\delta F}{\delta \psi} \right) \frac{\partial}{\partial x^j} \left(\frac{\delta G}{\delta \psi} \right) + 2\delta^{ij} \frac{\partial}{\partial y^i} \left(\frac{\delta F}{\delta \psi} \right) \frac{\partial}{\partial y^j} \left(\frac{\delta G}{\delta \psi} \right) \right] \\ &= - \left\langle \frac{\delta F}{\delta \psi}, \frac{\partial}{\partial x^i} \left(\delta^{ij} \psi \frac{\partial}{\partial x^j} \left(\frac{\delta G}{\delta \psi} \right) \right) + 2 \frac{\partial}{\partial y^i} \left(\delta^{ij} \psi \frac{\partial}{\partial y^j} \left(\frac{\delta G}{\delta \psi} \right) \right) \right\rangle. \end{aligned} \quad (3.28)$$

This type of dissipation bracket coming from a metric allows us to write the evolution of ψ as a “Liouville equation” $\dot{\psi} + \nabla_x \cdot (\dot{x}\psi) + \nabla_y \cdot (\dot{y}\psi) = 0$, since the extra terms it produces can be factored into some “flow velocity” in configuration space, proportional to the gradient of the free energy per bead-spring pair $\delta H / \delta \psi$.

For $H = H_{fluids}[\mathbf{m}, \rho] + H_s[\psi]$, the equation of motion for ψ is

$$\dot{\psi} + \frac{\partial}{\partial x^i} (u^i \psi) + \frac{\partial}{\partial y^i} \left(\frac{\partial u^i}{\partial x^j} y^j \psi \right) = \frac{1}{\zeta} \left[\frac{\partial}{\partial x^i} \left(\delta^{ij} \psi \frac{\partial}{\partial x^j} \left(\frac{\delta H_s}{\delta \psi} \right) \right) + 2 \frac{\partial}{\partial y^i} \left(\delta^{ij} \psi \frac{\partial}{\partial y^j} \left(\frac{\delta H_s}{\delta \psi} \right) \right) \right], \quad (3.29)$$

and $H_s[\psi]$ should now be interpreted as the free energy associated with the bead-spring pairs.

The dissipation bracket (3.28) implements bead-bead interactions, since it couples $H_s[\psi]$ to ψ , but does not add any extra coupling between \mathbf{m} and ψ . As there are no extra fluid-bead couplings, the force on the fluid due to the suspension as calculated with the semidirect product Lie–Poisson formulation is still valid.

The dissipation bracket (3.28) relates the non-conservative part of the Fokker–Planck equation and the gradient of the free energy using a linear mobility relation. More sophisticated mobility relations can be implemented by modifying the dissipation bracket [2]. One possible effect is the *hydrodynamic interaction* between the beads. This can be done by using a slightly different dissipation bracket. On \mathbb{R}^3 , let

$$(F, G)_D = \int d^3 x d^3 y \, \psi \left[\delta^{ij} \frac{\partial}{\partial x^i} \left(\frac{\delta F}{\delta \psi} \right) \frac{\partial}{\partial x^j} \left(\frac{\delta G}{\delta \psi} \right) + 2D^{ij}(y) \frac{\partial}{\partial y^i} \left(\frac{\delta F}{\delta \psi} \right) \frac{\partial}{\partial y^j} \left(\frac{\delta G}{\delta \psi} \right) \right], \quad (3.30)$$

where $D^{ij}(y) = \delta^{ij} + \gamma\Omega^{ij}$ for some parameter γ related to the size of the beads. The quantity $\Omega^{ij} = (|y|^2 \delta^{ij} + y^i y^j) / |y|^3$ is the *Oseen–Burgers tensor*, which describes the disturbance flow field around a small

sphere in a Stokes flow [18]. The extra terms obtained from using the dissipation bracket $(\cdot, \cdot)_D$ describes the advection of a bead by the disturbance flow field of the other bead.

Unfortunately, this bracket poses a considerable complication to the theory. There is no known way obtain a reduced system for y -moments of ψ that are sufficient to describe the stress state, even for Hookean springs. This property is commonly called (finite and exact) *closure* [28]. Ad hoc techniques such as “pre-averaging” have been used to obtain an effective mobility relation [3].

The dissipation bracket can also implement the *Newtonian viscous stress* on the fluid, by including an additional term in the dissipation bracket which is bilinear positive semidefinite in $\partial/\partial x^i(\delta F/\delta m_j)$ and $\partial/\partial x^i(\delta G/\delta m_j)$ with no ψ -dependence [1, 2, 9, 24]. It is typical in rheological applications to consider the bead-spring pairs to be suspended in a Newtonian fluid, so that the mechanism that moves the beads is Stokes drag. The *elastic particle-contributed stress*, which is the back-reaction on the fluid from doing work to the bead-spring pairs, is energy conserving. The purely dissipative Newtonian viscous stress, which comes from friction between adjacent fluid parcels, is a separate effect and does not affect the particle-contributed stress. Since we focus on the evolution equation for the distribution function ψ and the elastic particle-contributed stress for the rest of the paper, we omit the Newtonian viscous stress term.

3.5 The upper-convected Maxwell model from double bracket dynamics

So far we have considered the Poisson and dissipation brackets that are suitable for describing the dynamics of a bead-spring pair suspension. We now specialise to certain forms of the Hamiltonian functional, and show that the upper-convected Maxwell model can be derived from this double bracket system. Consider an isothermal fluid, with its temperature held at a fixed constant T throughout. As before, we postulate a Hamiltonian functional of the form $H = H_{fluids}[\mathbf{m}, \rho] + H_s[\psi]$, where H_{fluids} is the usual ideal compressible fluid Hamiltonian (3.17), and $H_s[\psi]$ is the free energy of the bead-spring pairs, given by

$$H_s[\psi] = \int d^n x d^n y (E(y)\psi + k_B T \psi \log(\psi)), \quad (3.31)$$

where k_B is the Boltzmann constant, and $E(y)$ is the internal energy of a bead-spring pair with bead-to-bead displacement y . This is a thermodynamic free energy $U - TS$, where

$$U[\psi] = \int d^n x d^n y E(y)\psi, \quad S[\psi] = -k_B \int d^n x d^n y \psi \log(\psi) \quad (3.32)$$

are the *internal energy* and the (*Boltzmann*) *entropy* of the distribution function ψ respectively.

The quantity $\log(\psi)$ is only uniquely specified up to a constant, since we are actually comparing $\psi d^n x d^n y$ to the standard volume element $d^n x d^n y$ in \mathbb{R}^{2n} , which is unique up to scaling. If we replace $d^n x d^n y$ with $\Lambda d^n x d^n y$ for some positive Λ , then $\log(\psi) \mapsto \log(\psi/\Lambda) = \log(\psi) - \log(\Lambda)$, and the Boltzmann entropy changes by

$$S[\psi] \mapsto S[\psi] + k_B \log(\Lambda) \int d^n x d^n y \psi. \quad (3.33)$$

Fortunately, the functional $N = \int d^n x d^n y \psi$ is a *Casimir functional* of the Lie–Poisson bracket. For any functional F , a direct computation shows that

$$\{F, N\} = - \left\langle \psi, \left(\frac{\delta F}{\delta \mathbf{m}} \right)^\# \cdot \mathbf{1} \right\rangle = 0. \quad (3.34)$$

Since $d(\delta N/\delta \psi) = 0$, $(F, N) = 0$ for all functionals F as well, so the dynamics are unaltered by such rescalings.

Now we can calculate the functional derivative of the free energy $H_s[\psi]$ in (3.31):

$$\frac{\delta H_s}{\delta \psi} = E(y) + k_B T (\log(\psi) + 1). \quad (3.35)$$

Substituting this into the equation for the force on the fluid gives

$$\mathcal{F}_i = \frac{\partial}{\partial x^i} \left(-2k_B T \int d^n y \psi \right) + \frac{\partial}{\partial x^j} \left(\int d^n y y^j \frac{\partial E}{\partial y^i} \psi \right) = \frac{\partial \sigma_i^j}{\partial x^j}, \quad (3.36)$$

where

$$\sigma_i^j = -2k_B T \int d^n y \psi \delta_i^j + \int d^n y y^j \frac{\partial E}{\partial y^i} \psi \quad (3.37)$$

is the *stress tensor* exerted on the fluid by the bead-spring pairs. The fact that the force can be written as the divergence of a stress tensor implies that linear momentum is conserved. This is related to the translational

invariance of the free energy $H_s[\psi]$ in (3.31). The evolution equation (3.29) for ψ becomes a *Fokker-Planck equation*:

$$\dot{\psi} + \frac{\partial}{\partial x^i} (u^i \psi) + \frac{\partial}{\partial y^i} \left(\frac{\partial u^i}{\partial x^j} y^j \psi \right) = \frac{2}{\zeta} \frac{\partial}{\partial y_i} \left(\delta^{ij} \frac{\partial E}{\partial y^j} \psi \right) + \frac{k_B T}{\zeta} (\nabla_x^2 \psi + 2 \nabla_y^2 \psi), \quad (3.38)$$

where $\nabla_x^2 = \delta^{ij} \partial^2 / \partial x^i \partial x^j$ and $\nabla_y^2 = \delta^{ij} \partial^2 / \partial y^i \partial y^j$. This coincides with the kinetic equation for bead-spring pairs with arbitrary internal energy $E(y)$ obtained in [3, 28], from a double bracket formulation.

There is no known general procedure to obtain closed evolution equations for the relevant moments of ψ appearing in the stress tensor for general $E(y)$. However, this is possible if the energy is quadratic, i.e. $E(y) = (\kappa/2) \delta_{ij} y^i y^j$, which will reproduce the upper-convected Maxwell model. Attempts in obtaining closed evolution equations for general $E(y)$ include the *Peterlin approximation*, which approximates the energy $E(y)$ as that of a Hookean spring, with an effective spring constant depending on the second y -moment of ψ [3, 28]. This approach produces nonlinear, but closed, evolution equations for the relevant moments of ψ .

Writing $\sigma^{jk} = \sigma_i^j \delta^{ik}$ for convenience, the stress tensor is

$$\sigma^{jk} = -2k_B T \delta^{jk} \int d^n y \psi + \kappa \int d^n y y^j y^k \psi = -2k_B T \delta^{jk} \langle 1 \rangle + \kappa \langle y^j y^k \rangle, \quad (3.39)$$

where $\langle \dots \rangle = \int d^n y \psi (\dots)$. Note that $\langle 1 \rangle = \int d^n y \psi = n(x)$ is the number density of bead-spring pairs in real space, and so it is not surprising that each bead in a pair contributes $n(x)k_B T$ to the isotropic pressure.

The evolution equation for the distribution function ψ is then

$$\dot{\psi} + \frac{\partial}{\partial x^i} (u^i \psi) + \frac{\partial}{\partial y^i} \left(\frac{\partial u^i}{\partial x^j} y^j \psi \right) = \frac{2\kappa}{\zeta} \frac{\partial}{\partial y^i} (y^i \psi) + \frac{k_B T}{\zeta} (\nabla_x^2 \psi + 2 \nabla_y^2 \psi). \quad (3.40)$$

Taking the 1 and $y^j y^k$ moments of (3.40) gives

$$\dot{\langle 1 \rangle} + \frac{\partial}{\partial x^i} (u^i \langle 1 \rangle) = \frac{k_B T}{\zeta} \nabla_x^2 \langle 1 \rangle, \quad (3.41)$$

$$\dot{\langle y^j y^k \rangle} + \frac{\partial}{\partial x^i} (u^i \langle y^j y^k \rangle) - \frac{\partial u^j}{\partial x^l} \langle y^l y^k \rangle - \frac{\partial u^k}{\partial x^l} \langle y^j y^l \rangle = -\frac{4\kappa}{\zeta} \langle y^j y^k \rangle + \frac{4k_B T}{\zeta} \delta^{jk} \langle 1 \rangle + \frac{k_B T}{\zeta} \nabla_x^2 \langle y^j y^k \rangle. \quad (3.42)$$

We can derive the upper-convected Maxwell model from (3.41, 3.42) as follows. Let $n = \langle 1 \rangle$ be the number density of bead-spring pairs, and $C^{jk} = \langle y^j y^k \rangle$ be the *conformation tensor*. Note that the stress tensor in (3.39) can be decomposed into two parts: $\sigma^{jk} = \sigma_{(0)}^{jk} + \sigma_{(1)}^{jk}$, where $\sigma_{(0)}^{jk} = -nk_B T \delta^{jk}$ is the pressure of suspended particles without internal structure. The stress due to internal structure $\sigma_{(1)}^{jk} = -nk_B T \delta^{jk} + \kappa C^{jk}$ evolves according to the following equation:

$$\dot{\sigma}_{(1)}^{jk} + \frac{\partial}{\partial x^i} (u^i \sigma_{(1)}^{jk}) - \frac{\partial u^j}{\partial x^l} \sigma_{(1)}^{lk} - \frac{\partial u^k}{\partial x^l} \sigma_{(1)}^{jl} = -\frac{4\kappa}{\zeta} \sigma_{(1)}^{jk} + nk_B T \left(\frac{\partial u^j}{\partial x^l} \delta^{lk} + \frac{\partial u^k}{\partial x^l} \delta^{jl} \right) + \frac{k_B T}{\zeta} \nabla_x^2 \sigma_{(1)}^{jk}, \quad (3.43)$$

which is the usual upper-convected Maxwell model, with an additional diffusion term. The diffusion term is usually absent because derivations often assume a separation of length scales: $|x| \gg |y|$, i.e. that the macroscopic fluid properties vary on length scales much larger than the length scale of the suspended bodies. We can adjust the factors in the metric (3.26) to make the x -diffusion term arbitrarily small relative to the other terms to reflect this separation of scales.

The equation (3.43) together with the momentum equation for the fluid form a closed system with a finite number of x -dependent fields. We can avoid solving for the full distribution function in the configuration space of suspensions because of this *finite closure*.

4 Higher order tangent bundles and semidirect product Lie algebra set-up for multibead-chains

In this section we describe the construction of the N^{th} order tangent bundle from a manifold, which can be considered as the configuration space of a small $(N+1)$ -bead chain [34]. This construction enjoys many analogous properties to the tangent bundle considered in section 3, which allows us to consider the advection of distribution functions for multibead-chains as semidirect product Lie-Poisson system.

4.1 The higher order tangent bundle $T^{(N)}M$

There are better finite-dimensional approximations to the space of all paths $\alpha : I \rightarrow M$, where as before I is some closed interval containing 0 in its interior. They can be constructed by taking the quotient under certain equivalence relations. Let α, β be paths, and x^i be local coordinates around $\alpha(0)$, so that $\alpha^i(t)$ are the coordinates of the path α . Then α is said to *have N^{th} order contact with β at $t = 0$* , written as $\alpha \stackrel{(N)}{\sim} \beta$, if and only if the $n(N+1)$ equations hold:

$$\alpha^i(0) = \beta^i(0), \quad \frac{d\alpha^i}{dt}(0) = \frac{d\beta^i}{dt}(0), \quad \frac{d^N \alpha^i}{dt^N}(0) = \frac{d^N \beta^i}{dt^N}(0). \quad (4.1)$$

Each of these equivalence classes is nonempty, since we can construct the local path $\alpha^i(t) = x^i + \sum_{a=1}^N \frac{t^a}{a!} y_{(a)}^i + O(t^{N+1})$ for arbitrary $x^i, y_{(1)}^i, \dots, y_{(N)}^i$. The space of all such equivalence classes is called the N^{th} order tangent bundle $T^{(N)}M$ of M , and is an $n(N+1)$ -dimensional manifold. The N^{th} order tangent bundle is also known as the *space of N -jets of \mathbb{R} into M with fixed source* and is sometimes denoted by $J_0^N(\mathbb{R}, M)$. The case $N = 1$ gives the usual tangent bundle from section 3.1. We use $(x^i, y_{(1)}^i, \dots, y_{(N)}^i)$ to denote the coordinates of a point in $T^{(N)}M$.

Informally, a point on the N^{th} order tangent bundle can be considered as an $(N+1)$ -point approximation to a small segment of a curve attached to M , using an N^{th} order Taylor polynomial. Note however that this is a local approximation to a smooth path based at a point – knowing the full Taylor series of a smooth path at one point is not in general sufficient to determine the value of the path at another arbitrarily close point. For example, the functions $f(t) = \exp(-1/t^2)$ and $f(t) = 0$ have the same Taylor series at $t = 0$.

4.2 Complete lifts of vector fields to $T^{(N)}M$

By adapting the same computation for how vector fields act on TM , we can allow vector fields to act on $T^{(N)}M$ in a natural way [34]. Let \mathbf{u} be a vector field on M . We construct a vector field $\mathbf{u}^\#$ on $T^{(N)}M$, called the *complete lift* of \mathbf{u} , as follows. Let $\alpha(t)$ be a path on M . The flow of \mathbf{u} by a small parameter s deforms the path to $\tilde{\alpha}(t, s)$ (see figure 1), whose components are

$$\tilde{\alpha}^i(t, s) = \alpha^i(t) + s u^i(\alpha(t)) + O(s^2). \quad (4.2)$$

Again, let

$$\begin{aligned} \tilde{x}^i(s) &= \tilde{\alpha}^i(0, s), \\ \tilde{y}_{(a)}^i(s) &= \left. \frac{\partial^a}{\partial t^a} \right|_{t=0} \tilde{\alpha}^i(t, s), \quad \text{for } a = 1, \dots, N. \end{aligned} \quad (4.3)$$

and denote their values at $s = 0$ as

$$\tilde{x}^i(0) = x^i, \quad \tilde{y}_{(a)}^i(0) = y_{(a)}^i \quad \text{for } a = 1, \dots, N. \quad (4.4)$$

If we apply $(\partial/\partial t)^a|_{t=0}$ to $\tilde{\alpha}(t, s)$ for $a = 1, \dots, N$, we obtain the following expressions:

$$\begin{aligned} \tilde{x}^i(s) &= x^i + s u^i(x) + O(s^2), \\ \tilde{y}_{(1)}^i(s) &= y_{(1)}^i + s \frac{\partial u^i}{\partial x^j}(x) y_{(1)}^j + O(s^2), \\ \tilde{y}_{(2)}^i(s) &= y_{(1)}^i + s \left(\frac{\partial^2 u^i}{\partial x^j \partial x^k}(x) y_{(1)}^j y_{(1)}^k + \frac{\partial u^i}{\partial x^j}(x) y_{(2)}^j \right) + O(s^2), \\ &\vdots \\ \tilde{y}_{(N)}^i(s) &= y_{(N)}^i + s \left(\frac{d^N}{dt^N} u^i(\alpha(t)) \right) \Big|_{t=0} + O(s^2). \end{aligned} \quad (4.5)$$

This flow, which is parametrised by s , defines a vector field $\mathbf{u}^\#$ on $T^{(N)}M$ called the *complete lift*. The components of $\mathbf{u}^\#$ relative to the coordinate system $(x^i, y_{(1)}^i, \dots, y_{(N)}^i)$ can be obtained from taking $(\partial/\partial s)|_{s=0}$ of the expressions above:

$$\mathbf{u}^\#(x, y_{(1)}, \dots, y_{(N)}) = \left(u^i(\alpha(0)), \frac{d}{dt} u^i(\alpha(t)) \Big|_{t=0}, \dots, \frac{d^N}{dt^N} u^i(\alpha(t)) \Big|_{t=0} \right), \quad (4.6)$$

$$\text{where } \alpha^i(t) = x^i + \sum_{a=1}^N \frac{t^a}{a!} y_{(a)}^i + O(t^{N+1}). \quad (4.7)$$

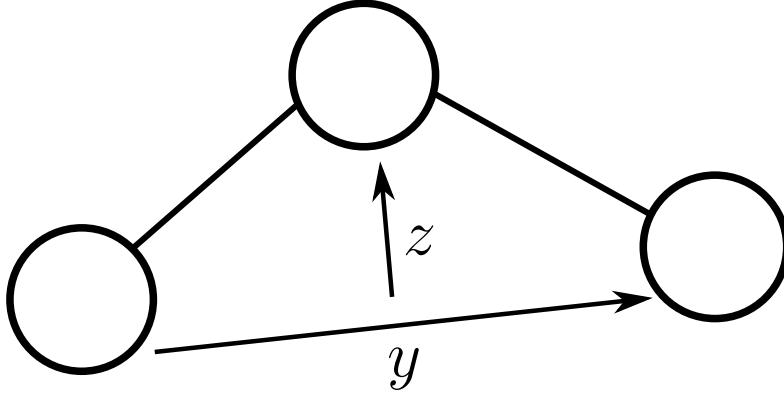


Figure 2: The coordinates y and z describe the internal degrees of freedom of the 3-bead chain.

Taylor expanding and comparing powers of t shows that the choice of the $O(t^{N+1})$ term will not affect the components of $\mathbf{u}^\#$.

The crucial property here is that the complete lift of vector fields is a Lie algebra homomorphism $\text{Vect}(M) \rightarrow \text{Vect}(T^{(N)}M)$, as

$$([\mathbf{u}, \mathbf{v}]_M)^\# = [\mathbf{u}^\#, \mathbf{v}^\#]_{T^{(N)}M}. \quad (4.8)$$

A sketch of proof is given in appendix A. The action of vector fields \mathbf{u} on M on smooth functions f on $T^{(N)}M$ given by $f \mapsto \mathbf{u}^\# \cdot f$ is a Lie algebra representation. Hence the corresponding semidirect product can be formed, with vector fields \mathbf{u} on M acting on functions f on $T^{(N)}M$ by the complete lift.

4.3 Subbracket for the distribution function in the semidirect product Lie algebra formulation

The semidirect product Lie algebra relevant to a compressible fluid advecting $(N+1)$ -bead chains is

$$\mathfrak{g}_s = \text{Vect}(M) \ltimes \left(C^\infty(M) \oplus C^\infty(T^{(N)}M) \right). \quad (4.9)$$

The smooth dual space to $C^\infty(T^{(N)}M)$ can be taken as the space of volume forms $\Omega^{n(N+1)}(T^{(N)}M)$, with typical element $\psi d^n x d^n y_{(1)} \dots d^n y_{(N)}$. So the smooth dual space \mathfrak{g}_s^* can be taken as $\text{Vect}(M)^* \oplus \Omega^n(M) \oplus \Omega^{n(N+1)}(T^{(N)}M)$. A typical element of \mathfrak{g}_s^* is a triple (\mathbf{m}, ρ, ψ) , where \mathbf{m} is the fluid momentum density, ρ is the fluid mass density, and ψ can be thought of as the distribution function on the configuration space of the $(N+1)$ -bead chains.

The minus Lie–Poisson bracket for functionals $F = F[\mathbf{m}, \rho, \psi]$ and $G = G[\mathbf{m}, \rho, \psi]$ is

$$\begin{aligned} \{F, G\}[\mathbf{m}, \rho, \psi] &= - \left\langle \mathbf{m}, \left[\frac{\delta F}{\delta \mathbf{m}}, \frac{\delta G}{\delta \mathbf{m}} \right] \right\rangle - \left\langle \rho, \frac{\delta F}{\delta \mathbf{m}} \cdot \frac{\delta G}{\delta \rho} - \frac{\delta G}{\delta \mathbf{m}} \cdot \frac{\delta F}{\delta \rho} \right\rangle - \left\langle \psi, \left(\frac{\delta F}{\delta \mathbf{m}} \right)^\# \cdot \frac{\delta G}{\delta \psi} - \left(\frac{\delta G}{\delta \mathbf{m}} \right)^\# \cdot \frac{\delta F}{\delta \psi} \right\rangle \\ &= \{F, G\}_{fluids} + \{F, G\}_\psi, \end{aligned} \quad (4.10)$$

where $\{F, G\}_{fluids}$ denotes the usual compressible fluid bracket, and $\{F, G\}_\psi$ denotes ψ -subbracket i.e. the terms that explicitly involve ψ .

5 The 3-bead chain model

As an application of the ideas of the previous section, consider the case $N = 2$. The second order tangent bundle $T^{(2)}M$ is the configuration space of a 3-bead chain. The extra degrees of freedom $y_{(1)} = y, y_{(2)} = z$ (renamed for notational clarity) can be thought of as the average extension and the bending of the chain, respectively, as shown in figure 2. Forming the semidirect product $\mathfrak{g}_s = \text{Vect}(M) \ltimes (C^\infty(M) \oplus C^\infty(T^{(2)}M))$ and looking at

the Lie–Poisson dynamics for functionals on the dual \mathfrak{g}_s^* , we obtain the ψ -subbracket as follows:

$$\begin{aligned}\{F, G\}_\psi &= - \left\langle \psi, \left(\frac{\delta F}{\delta \mathbf{m}} \right)^\# \cdot \frac{\delta G}{\delta \psi} - \left(\frac{\delta G}{\delta \mathbf{m}} \right)^\# \cdot \frac{\delta F}{\delta \psi} \right\rangle \\ &= - \int d^n x d^n y d^n z \left[\psi \left[\frac{\delta F}{\delta m_i} \frac{\partial}{\partial x^i} \left(\frac{\delta G}{\delta \psi} \right) + \frac{\partial}{\partial x^j} \left(\frac{\delta F}{\delta m_i} \right) y^j \frac{\partial}{\partial y^i} \left(\frac{\delta G}{\delta \psi} \right), \right. \right. \\ &\quad + \left(\frac{\partial^2}{\partial x^j \partial x^k} \left(\frac{\delta F}{\delta m_i} \right) y^j y^k + \frac{\partial}{\partial x^j} \left(\frac{\delta F}{\delta m_i} \right) z^j \right) \frac{\partial}{\partial z^i} \left(\frac{\delta G}{\delta \psi} \right) \\ &\quad - \frac{\delta G}{\delta m_i} \frac{\partial}{\partial x^i} \left(\frac{\delta F}{\delta \psi} \right) + \frac{\partial}{\partial x^j} \left(\frac{\delta G}{\delta m_i} \right) y^j \frac{\partial}{\partial y^i} \left(\frac{\delta F}{\delta \psi} \right) \\ &\quad \left. - \left(\frac{\partial^2}{\partial x^j \partial x^k} \left(\frac{\delta G}{\delta m_i} \right) y^j y^k + \frac{\partial}{\partial x^j} \left(\frac{\delta G}{\delta m_i} \right) z^j \right) \frac{\partial}{\partial z^i} \left(\frac{\delta F}{\delta \psi} \right) \right].\end{aligned}\quad (5.1)$$

If we consider Hamiltonians of the form $H = H_{fluids}[\mathbf{m}, \rho] + H_s[\psi]$ and let $\mathbf{u} = \delta H / \delta \mathbf{m}$, then the evolution equation for ψ and the extra force \mathcal{F}_i on the fluid are respectively

$$\dot{\psi} = - \frac{\partial}{\partial x^i} (u^i \psi) - \frac{\partial}{\partial y^i} \left(\frac{\partial u^i}{\partial x^j} y^j \psi \right) - \frac{\partial}{\partial z^i} \left(\left[\frac{\partial^2 u^i}{\partial x^j \partial x^k} y^j y^k + \frac{\partial u^i}{\partial x^j} z^j \right] \psi \right), \quad (5.2)$$

$$\begin{aligned}\mathcal{F}_i &= \int d^n y d^n z \left[- \frac{\partial}{\partial x^i} \left(\frac{\delta H_s}{\delta \psi} \right) + \frac{\partial}{\partial x^j} \left(y^j \frac{\partial}{\partial y^i} \left(\frac{\delta H_s}{\delta \psi} \right) \right) \right. \\ &\quad \left. + \frac{\partial}{\partial x^j} \left(z^j \frac{\partial}{\partial z^i} \left(\frac{\delta H_s}{\delta \psi} \right) \right) - \frac{\partial^2}{\partial x^j \partial x^k} \left(y^j y^k \frac{\partial}{\partial z^i} \left(\frac{\delta H_s}{\delta \psi} \right) \right) \right].\end{aligned}\quad (5.3)$$

This is obtained by the usual procedure of equating

$$\dot{F} = \left\langle \frac{\delta F}{\delta \mathbf{m}}, \dot{\mathbf{m}} \right\rangle + \left\langle \frac{\delta F}{\delta \rho}, \dot{\rho} \right\rangle + \left\langle \frac{\delta F}{\delta \psi}, \dot{\psi} \right\rangle = \{F, H\} = \{F, H\}_{fluids} + \{F, H\}_\psi \quad (5.4)$$

for arbitrary F , and collecting the terms proportional to $\delta F / \delta \mathbf{m}$ and $\delta F / \delta \psi$ respectively due to the ψ -subbracket, after some integrations by parts.

The term $(\partial^2 u^i / \partial x^j \partial x^k) y^j y^k$ in (5.2) can be thought of as the *bending rate* of the bead chain due to a difference between the stretching velocities across the bead chain. The suspension couples to the second derivative of the flow velocity \mathbf{u} , so it can detect *vorticity gradients* across the flow. As we shall demonstrate in section 5.2, this model supports a force term \mathcal{F}_i with nonzero torque i.e. the stress tensor can be non-symmetric [4, 5]. If we drop this term, the kinematics reduces to the conventional Rouse model [3], where the multibead-chains are affected by the local velocity gradient by not any higher derivatives.

In more geometrical terms, the flow vector field \mathbf{u} will be acting on the configuration space $(T \oplus T)M$ instead of $T^{(2)}M$ without the second derivative term. Each point in $(T \oplus T)M$ consists of a pair of tangent vectors at a point on M . Figures 3 and 4 illustrate the differences graphically. As a consequence, the resulting semidirect product Lie–Poisson bracket constructed using $(T \oplus T)M$ is different from that constructed using $T^{(2)}M$. This difference is difficult to see if we only consider the configuration space itself but not how it is constructed. For example, when $M = \mathbb{R}^n$, both $(T \oplus T)M$ and $T^{(2)}M$ are diffeomorphic too \mathbb{R}^{3n} . We can construct an isomorphism of $(T \oplus T)M$ and $T^{(2)}M$ as fibre bundles using a metric – see appendix B.1. However, the isomorphism depends on the metric, and the complete lifts of vector fields to $(T \oplus T)M$ and $T^{(2)}M$ respectively do not coincide under the isomorphism.

This difference leads to some qualitatively different physical behaviour. As we shall see in section 5.1, the Hookean 3-bead chain suspension has an *asymmetric* stress tensor due to the “back-reaction” to the second derivative term $(\partial^2 u^i / \partial x^j \partial x^k) y^j y^k$. This term is formally of order $|y|/|x|$ smaller than the other terms in the evolution equation for ψ (5.2), where $|y|$ is the legnthscale of the chain and $|x|$ is the gradient scale of the flow. One recovers the Rouse model by dropping this term.

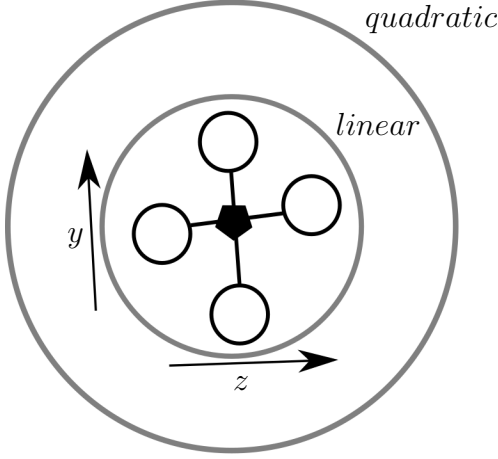


Figure 3: $(T \oplus T)M$ consists of a point on M , and a pair of tangent vectors y, z attached to that point. It can be thought of as the configuration space of two bead-spring pairs with a common centre.

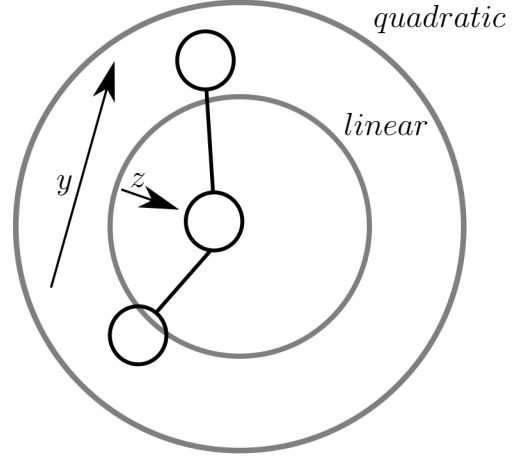


Figure 4: $T^{(2)}M$ consists of equivalence classes of paths $I \rightarrow M$ with the same Taylor series up to second order, with y, z being the first and second order coefficients in the Taylor expansion respectively. It can be thought of as the configuration space of a 3-bead chain.

5.1 Dissipation bracket for 3-bead chains

Following the example of the bead-spring pairs, we construct the dissipation bracket for the 3-bead chain suspension. Let $M = \mathbb{R}^n$, so we can identify $T^{(2)}M$ with \mathbb{R}^{3n} with coordinates (x^i, y^i, z^i) . Consider the usual Riemannian metric g on \mathbb{R}^{3n} , which can be written as

$$ds^2 = \delta_{ij} dx^i dx^j + \delta_{ij} dy^i dy^j + \delta_{ij} dz^i dz^j. \quad (5.5)$$

The construction of Riemannian metrics on higher order tangent bundles of general Riemannian manifolds is considered in appendix B.

We define the dissipation bracket

$$(F, G) = \int d^n x d^n y d^n z \, \psi \, \tilde{g} \left(d \left(\frac{\delta F}{\delta \psi} \right), d \left(\frac{\delta G}{\delta \psi} \right) \right), \quad (5.6)$$

where \tilde{g} denotes the inverse of g . The coordinate expression for the dissipation bracket is

$$(F, G) = \int d^n x d^n y d^n z \, \psi \left[\delta^{ij} \frac{\partial}{\partial x^i} \left(\frac{\delta F}{\delta \psi} \right) \frac{\partial}{\partial x^j} \left(\frac{\delta F}{\delta \psi} \right) + \delta^{ij} \frac{\partial}{\partial y^i} \left(\frac{\delta F}{\delta \psi} \right) \frac{\partial}{\partial y^j} \left(\frac{\delta F}{\delta \psi} \right) + \delta^{ij} \frac{\partial}{\partial z^i} \left(\frac{\delta F}{\delta \psi} \right) \frac{\partial}{\partial z^j} \left(\frac{\delta F}{\delta \psi} \right) \right]. \quad (5.7)$$

The dynamics is then given by

$$\dot{F} = \{F, H\} - \frac{1}{\zeta} (F, H), \quad (5.8)$$

for some positive parameter $1/\zeta$ called the *mobility*. This dissipation bracket provides an implementation of a linear mobility relation between the applied force and the relative velocity to the surrounding fluid.

The functional H should now be interpreted as a free energy. As a generalisation to (3.31), consider free energies of the form

$$H_s[\psi] = \int d^n x d^n y d^n z \, (E(y, z) \psi + k_B T \psi \log \psi), \quad (5.9)$$

with variational derivative $\delta H_s / \delta \psi = E(y, z) + k_B T (\log \psi + 1)$. The force can be written as the divergence of a stress tensor, $\mathcal{F}_i = \partial \sigma_i^j / \partial x^j$ in (5.3), where

$$\sigma_i^j = -3k_B T \int d^n y d^n z \, \psi + \int d^n y d^n z \, \psi \left(y^j \frac{\partial E}{\partial y^j} + z^j \frac{\partial E}{\partial z^j} \right) - \frac{\partial}{\partial x^k} \int d^n y d^n z \, \psi y^j y^k \frac{\partial E}{\partial z^k}. \quad (5.10)$$

The evolution equation for ψ is obtained similarly:

$$\begin{aligned} \dot{\psi} + \frac{\partial}{\partial x^i} (u^i \psi) + \frac{\partial}{\partial y^i} \left(\frac{\partial u^i}{\partial x^j} y^j \psi \right) + \frac{\partial}{\partial z^i} \left(\left[\frac{\partial^2 u^i}{\partial x^j \partial x^k} y^j y^k + \frac{\partial u^i}{\partial x^j} z^j \right] \psi \right) \\ = \frac{1}{\zeta} \frac{\partial}{\partial y^i} \left(\delta^{ij} \frac{\partial E}{\partial y^j} \psi \right) + \frac{1}{\zeta} \frac{\partial}{\partial z^i} \left(\delta^{ij} \frac{\partial E}{\partial z^j} \psi \right) + \frac{k_B T}{\zeta} (\nabla_x^2 \psi + \nabla_y^2 \psi + \nabla_z^2 \psi), \end{aligned} \quad (5.11)$$

where $\nabla_x^2 = \delta^{ij} \partial^2 / \partial x^i \partial x^j$, $\nabla_y^2 = \delta^{ij} \partial^2 / \partial y^i \partial y^j$, and $\nabla_z^2 = \delta^{ij} \partial^2 / \partial z^i \partial z^j$.

For general forms of $E(y, z)$, there is no known exact method to express the evolution of the relevant moments appearing in the stress tensor in terms of a finite set of moments in ψ , i.e. there is no finite closure in general. However, a finite closure exists for a quadratic energy of the form

$$E(y, z) = \frac{\kappa_1}{2} \delta_{ij} y^i y^j + \frac{\kappa_2}{2} \delta_{ij} z^i z^j. \quad (5.12)$$

By writing $\sigma^{jk} = \sigma_i^j \delta^{ik}$ and using the notation $\langle \dots \rangle = \int d^n y d^n z \psi(\dots)$, we can write the stress tensor (5.10) as

$$\sigma^{jk} = -3k_B T \langle 1 \rangle \delta^{jk} + \kappa_1 \langle y^j y^k \rangle + \kappa_2 \langle z^j z^k \rangle - \kappa_2 \frac{\partial}{\partial x^l} \langle y^j y^l z^k \rangle. \quad (5.13)$$

The evolution equation (5.11) for ψ then simplifies to

$$\begin{aligned} \dot{\psi} + \frac{\partial}{\partial x^i} (u^i \psi) + \frac{\partial}{\partial y^i} \left(\frac{\partial u^i}{\partial x^j} y^j \psi \right) + \frac{\partial}{\partial z^i} \left(\left[\frac{\partial^2 u^i}{\partial x^j \partial x^k} y^j y^k + \frac{\partial u^i}{\partial x^j} z^j \right] \psi \right) \\ = \frac{1}{\zeta} \frac{\partial}{\partial y^i} (y^i \psi) + \frac{1}{\zeta} \frac{\partial}{\partial z^i} (z^i \psi) + \frac{k_B T}{\zeta} (\nabla_x^2 \psi + \nabla_y^2 \psi + \nabla_z^2 \psi). \end{aligned} \quad (5.14)$$

The stress tensor σ^{jk} in (5.13) is not manifestly symmetric, but the system nonetheless conserves total fluid angular momentum. The torque of the suspension on the fluid is the antisymmetric part of the stress tensor: $\tau^{jk} = \sigma^{jk} - \sigma^{kj}$. For this specific form of σ^{jk} , the torque τ^{jk} is a divergence of a 3-index tensor. This means the torque terms are not sources or sinks of angular momentum, but *angular momentum fluxes* [4]. These extra angular momentum fluxes can be thought of as the transmission of angular momentum between adjacent fluid parcels across a common material surface, through the bending of chains that cross the surface. Since the chain has no inertia, the torques on the chain must balance at all times, which means the transmission of angular momentum is instantaneous.

There is a slightly different description of this asymmetric stress tensor in terms of generalised continuum systems that can possibly have internal angular momentum, such as polar fluids [4, 29]. These generalised continuum systems were first considered by Cosserat and Cosserat [5]. The rate of change of total angular momentum in a Lagrangian control volume consists of sources such as body forces and body torques, as well as fluxes through the boundary of the control volume. There are two types of angular momentum fluxes, the first being the *hydrodynamic angular momentum flux* $-\sigma \times \mathbf{x}$, which is the angular momentum flux generated by the fluid stress, and the second being a *couple stress*, an angular momentum flux generated by the interaction of the internal degrees of freedom. The couple stress depends on the intrinsic properties of the fluid, in the same way the hydrodynamic stress depends on the thermodynamic equation of state, viscosity etc. of the fluid. The hydrodynamic torque $\mathbf{x} \times \nabla \cdot \sigma$ can be separated into two parts

$$\mathbf{x} \times \nabla \cdot \sigma = -\nabla \cdot (\sigma \times \mathbf{x}) - \tau, \quad (5.15)$$

where the first term $-\nabla \cdot (\sigma \times \mathbf{x})$ is the divergence of the hydrodynamic angular momentum flux, and the second term τ is (up to conventions on the sign and factors of 2) the antisymmetric (or pseudovector) part of the hydrodynamic stress tensor σ . The hydrodynamic torque is not necessarily the divergence of the hydrodynamic angular momentum flux, and the “excess” term τ represents the exchange of angular momentum between the internal and fluid degrees of freedom.

In our system of Hookean 3-bead chains, there are no body forces or body torques. Moreover, since the 3-bead chains are immersed in a Stokes flow, they have no inertia and hence no internal angular momentum. So there is instantaneous torque balance – the “excess” term τ , which is the antisymmetric part of the hydrodynamic stress tensor σ , must be balanced by the divergence of a couple stress. In our case, τ is an exact divergence, so we can identify τ with (the negative of) the couple stress. This is different from systems with internal “spin” degrees of freedom such as ferrofluids, where the couple stress alone cannot balance the “excess” term in (or antisymmetric part of) the hydrodynamic stress [29, 31].

The Hookean 3-bead chain model with dissipation terms conserves linear and angular momentum. This is consistent with *Noether’s theorem*, since the energy $E(y, z)$ in (5.12) is translationally and rotationally invariant.

Moreover, since the linear and angular momentum do not depend on ψ , they are not affected by the dissipation bracket, so the double bracket system as a whole conserves linear and angular momentum.

If we apply $\int d^n z$ to the evolution equation (5.14) of ψ , we obtain the previous evolution equation (3.38) for the bead-spring pairs, up to numerical factors in the dissipation bracket. This is analogous to “forgetting” the middle bead.

As we shall see in the next section, the moments appearing in the stress tensor (5.13) do not quite form a closed system, but this can be fixed by including a few extra moments.

5.2 Closure of the 3-bead chain model with quadratic energy

By a finite and exact *closure* we mean that there is a finite set of moments μ_1, \dots, μ_I of ψ , i.e. quantities of the form $\langle p(y, z) \rangle$ for a polynomial p , such that the evolution of each moment can be expressed using this set of moments, together with \mathbf{u} and its spatial derivatives:

$$\dot{\mu}_J = f_J(\mu_1, \dots, \mu_I; \mathbf{u}) \quad \text{for } J = 1, \dots, I, \quad (5.16)$$

and such that $\sigma = \sigma(\mu_1, \dots, \mu_I; \mathbf{u})$ i.e. the stress tensor is completely described by these moments.

We show explicitly that the 3-bead chain model with quadratic energy, described by the equations (5.13, 5.14,) has such a closure. Since $\langle 1 \rangle, \langle y^j y^k \rangle, \langle z^j z^k \rangle, \langle y^i y^l z^k \rangle$ all appear in the expression for σ^{jk} , let us look at their time derivatives:

$$\langle \dot{1} \rangle + \frac{\partial}{\partial x^i} (u^i \langle 1 \rangle) = \frac{k_B T}{\zeta} \nabla_x^2 \langle 1 \rangle, \quad (5.17)$$

$$\begin{aligned} \langle \dot{y^j y^k} \rangle + \frac{\partial}{\partial x^i} (u^i \langle y^j y^k \rangle) - \frac{\partial u^j}{\partial x^l} \langle y^l y^k \rangle - \frac{\partial u^k}{\partial x^l} \langle y^j y^l \rangle \\ = -\frac{2\kappa_1}{\zeta} \langle y^j y^k \rangle + \frac{2k_B T}{\zeta} \delta^{jk} \langle 1 \rangle + \frac{k_B T}{\zeta} \nabla_x^2 \langle y^j y^k \rangle, \end{aligned} \quad (5.18)$$

$$\begin{aligned} \langle \dot{z^j z^k} \rangle + \frac{\partial}{\partial x^i} (u^i \langle z^j z^k \rangle) - \frac{\partial u^j}{\partial x^l} \langle z^l z^k \rangle - \frac{\partial u^k}{\partial x^l} \langle z^j z^l \rangle - \frac{\partial^2 u^j}{\partial x^m \partial x^l} \langle y^m y^l z^k \rangle - \frac{\partial^2 u^k}{\partial x^m \partial x^l} \langle y^m y^l z^j \rangle \\ = -\frac{2\kappa_2}{\zeta} \langle z^j z^k \rangle + \frac{2k_B T}{\zeta} \delta^{jk} \langle 1 \rangle + \frac{k_B T}{\zeta} \nabla_x^2 \langle z^j z^k \rangle, \end{aligned} \quad (5.19)$$

$$\begin{aligned} \langle \dot{y^j y^l z^k} \rangle + \frac{\partial}{\partial x^i} (u^i \langle y^j y^l z^k \rangle) - \frac{\partial u^j}{\partial x^m} \langle y^m y^l z^k \rangle - \frac{\partial u^l}{\partial x^m} \langle y^j y^m z^k \rangle - \frac{\partial u^k}{\partial x^m} \langle y^j y^l z^m \rangle - \frac{\partial^2 u^k}{\partial x^m \partial x^n} \langle y^m y^n y^j y^l \rangle \\ = -\frac{2\kappa_1}{\zeta} \langle y^j y^l z^k \rangle - \frac{\kappa_2}{\zeta} \langle y^j y^l z^k \rangle + \frac{2k_B T}{\zeta} \delta^{jl} \langle z^k \rangle + \frac{k_B T}{\zeta} \nabla_x^2 \langle y^j y^l z^k \rangle. \end{aligned} \quad (5.20)$$

The moments $\langle 1 \rangle, \langle y^j y^k \rangle, \langle z^j z^k \rangle, \langle y^i y^l z^k \rangle$ do not quite form a closed system, as their time evolution depends on the extra moments $\langle y^m y^n y^j y^l \rangle$ and $\langle z^k \rangle$. However, including the time evolution of just these extra moments closes the system:

$$\begin{aligned} \langle \dot{y^m y^n y^j y^l} \rangle + \frac{\partial}{\partial x^i} (u^i \langle y^m y^n y^j y^l \rangle) - \frac{\partial u^m}{\partial x^i} \langle y^i y^n y^j y^l \rangle - \frac{\partial u^n}{\partial x^i} \langle y^m y^i y^j y^l \rangle - \frac{\partial u^j}{\partial x^i} \langle y^m y^n y^i y^l \rangle - \frac{\partial u^l}{\partial x^i} \langle y^m y^n y^j y^i \rangle \\ = -\frac{4\kappa_1}{\zeta} \langle y^m y^n y^j y^l \rangle + \frac{k_B T}{\zeta} \nabla_x^2 \langle y^m y^n y^j y^l \rangle \\ + \frac{2k_B T}{\zeta} (\delta^{mn} \langle y^j y^l \rangle + \delta^{mj} \langle y^n y^l \rangle + \delta^{ml} \langle y^n y^j \rangle + \delta^{nj} \langle y^m y^l \rangle + \delta^{nl} \langle y^m y^j \rangle + \delta^{jl} \langle y^m y^n \rangle), \end{aligned} \quad (5.21)$$

$$\langle \dot{z^k} \rangle + \frac{\partial}{\partial x^i} (u^i \langle z^k \rangle) - \frac{\partial u^k}{\partial x^i} \langle z^i \rangle - \frac{\partial^2 u^k}{\partial x^m \partial x^n} \langle y^m y^n \rangle = -\frac{\kappa_2}{\zeta} \langle z^k \rangle + \frac{k_B T}{\zeta} \nabla_x^2 \langle z^k \rangle. \quad (5.22)$$

Thus the moments $\langle 1 \rangle, \langle y^j y^k \rangle, \langle z^j z^k \rangle, \langle y^i y^l z^k \rangle, \langle y^m y^n y^j y^l \rangle, \langle z^k \rangle$ form a closed system of evolution equations given the flow field \mathbf{u} , and are also sufficient to describe the stress tensor σ^{jk} in (5.13) completely. It is possible to interpret these moments as tensor fields – see appendix B for more details.

The Hookean 3-bead chain model describes suspensions of molecules with stretching and bending degrees of freedom. This type of suspension can transmit angular momentum between adjacent fluid parcels. We will study this model under a shear flow in a sequel paper.

6 Explicit formulae for the multibead-chain model

Having investigated the 3-bead chain as an example, we now return to the general case. In section 4 we have considered the action of vector fields $\mathbf{u} \in \text{Vect}(M)$ on functions on the N^{th} order tangent bundle $T^{(N)}M$, which is

the configuration space of small $(N+1)$ -bead chains living on a manifold M . We also considered the semidirect product relevant to the advection of such multibead chains in an ideal compressible fluid, and obtained the following semidirect Lie–Poisson bracket. Let (\mathbf{m}, ρ, ψ) denote the fluid momentum density, fluid mass density, and the distribution function of multibead-chains in configuration space, respectively. For functionals F, G , their Poisson bracket is

$$\begin{aligned} \{F, G\}[\mathbf{m}, \rho, \psi] &= - \left\langle \mathbf{m}, \left[\frac{\delta F}{\delta \mathbf{m}}, \frac{\delta G}{\delta \mathbf{m}} \right] \right\rangle - \left\langle \rho, \frac{\delta F}{\delta \mathbf{m}} \cdot \frac{\delta G}{\delta \rho} - \frac{\delta G}{\delta \mathbf{m}} \cdot \frac{\delta F}{\delta \rho} \right\rangle - \left\langle \psi, \left(\frac{\delta F}{\delta \mathbf{m}} \right)^\# \cdot \frac{\delta G}{\delta \psi} - \left(\frac{\delta G}{\delta \mathbf{m}} \right)^\# \cdot \frac{\delta F}{\delta \psi} \right\rangle, \\ &= \{F, G\}_{fluids} + \{F, G\}_\psi, \end{aligned} \quad (6.1)$$

where $\{F, G\}_{fluids}$ denotes the usual compressible fluid bracket, and the subbracket $\{F, G\}_\psi$ denotes the terms that explicitly involve ψ .

We work exclusively in coordinates and take $M = \mathbb{R}^n$ in the following. Let x^i be coordinates on M and $(x^i, y_{(1)}^i, \dots, y_{(N)}^i)$ be the induced coordinates on $T^{(N)}M$. We denote the standard volume element in the space of the “internal degrees of freedom” with respect to this coordinate system as

$$d\Gamma = d^n y_{(1)} \cdots d^n y_{(N)}. \quad (6.2)$$

To write the components of the complete lift $\mathbf{u}^\#$ in terms of the components of $\mathbf{u}(x)$ and its derivatives, we define the *exponential* of an operator X by the formal power series $\exp(X) = 1 + X + X^2/2! + \dots$, and write

$$u^i(x + \delta x) = \exp \left(\delta x^j \frac{\partial}{\partial x^j} \right) u^i(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\delta x^j \frac{\partial}{\partial x^j} \right)^n u^i(x). \quad (6.3)$$

We only need a finite number of terms in the series in the following. In particular, the convergence of the series is not an issue for our later arguments.

The components of $\mathbf{u}^\#$ in the coordinate system $(x^i, y_{(1)}^i, \dots, y_{(N)}^i)$ can be written as $(u^i, u_{(1)}^i, \dots, u_{(N)}^i)$, where

$$\begin{aligned} u_{(a)}^i &= \left(\frac{\partial}{\partial t} \right)^a \Big|_{t=0} u^i \left(x + \sum_{b=1}^N \frac{t^b}{b!} y_{(b)} \right), \\ &= \left(\frac{\partial}{\partial t} \right)^a \left[\exp \left(\sum_{b=1}^N \frac{t^b}{b!} y_{(b)}^j \frac{\partial}{\partial x^j} \right) \right]_{t=0} \cdot u^i(x), \\ &= \mathcal{P}_a \left(y_{(1)}, \dots, y_{(N)}, \frac{\partial}{\partial x} \right) \cdot u^i(x). \end{aligned} \quad (6.4)$$

The expressions \mathcal{P}_a are defined to be the a^{th} t -derivative of the exponential operator in the second line of (6.4). We can equivalently characterise \mathcal{P}_a in terms of a generating function

$$\exp \left(\sum_{b=1}^N \frac{t^b}{b!} y_{(b)}^j \frac{\partial}{\partial x^j} \right) = 1 + \sum_{a=1}^N \frac{t^a}{a!} \mathcal{P}_a \left(y_{(1)}, \dots, y_{(N)}, \frac{\partial}{\partial x} \right) + O(t^{N+1}). \quad (6.5)$$

Collecting powers of t in the exponential series shows that \mathcal{P}_a is a polynomial in the *commuting* variables $y_{(1)}, \dots, y_{(N)}, \partial/\partial x$. We write $\mathcal{P}_a = \mathcal{P}_a(y, \partial/\partial x)$ to indicate its dependence on the y -coordinates, and emphasise that it is a differential operator acting on quantities with x -dependence.

We verify a few crucial properties of \mathcal{P}_a by collecting powers of t in (6.5):

- (i) a is the highest power of $\partial/\partial x$ appearing \mathcal{P}_a .
- (ii) 1 is the lowest power of $\partial/\partial x$ appearing \mathcal{P}_a . This means there is no “constant term” in \mathcal{P}_a as a polynomial in $\partial/\partial x$, which is a fact we use later to express the force as the divergence of a stress tensor for some specific forms of the Hamiltonian functional.
- (iii) Define the *order* of each monomial in $y_{(1)}, \dots, y_{(N)}$ to be the sum of its subscripts, and the *order* of a polynomial $p(y)$ as the maximum order of its monomial terms. We also say a polynomial $p(y)$ is (*weighted*) *homogeneous of order b* if the scaling $y_{(a)} \mapsto \lambda^a y_{(a)}$ sends $p(y) \mapsto \lambda^b p(y)$. Then \mathcal{P}_a is a polynomial of order a in the variables $y_{(1)}, \dots, y_{(N)}$ with coefficients in $\partial/\partial x$. In particular, \mathcal{P}_a does not depend on $y_{(b)}$ for $b > a$. We will return to this property when we consider the problem of exact closure.

We can thus write the ψ -subbracket of functionals F, G on (\mathbf{m}, ρ, ψ) as

$$\begin{aligned}
\{F, G\}_\psi &= - \int d^n x d\Gamma \, \psi \left[\frac{\delta F}{\delta m_i} \frac{\partial}{\partial x^i} \left(\frac{\delta G}{\delta \psi} \right) - \frac{\delta G}{\delta m_i} \frac{\partial}{\partial x^i} \left(\frac{\delta F}{\delta \psi} \right) \right] \\
&\quad - \int d^n x d\Gamma \, \psi \sum_{a=1}^N \left(\mathcal{P}_a \left(y, \frac{\partial}{\partial x} \right) \cdot \frac{\delta F}{\delta m_i} \right) \left(\frac{\partial}{\partial y_{(a)}^i} \frac{\delta G}{\delta \psi} \right) \\
&\quad + \int d^n x d\Gamma \, \psi \sum_{a=1}^N \left(\mathcal{P}_a \left(y, \frac{\partial}{\partial x} \right) \cdot \frac{\delta G}{\delta m_i} \right) \left(\frac{\partial}{\partial y_{(a)}^i} \frac{\delta F}{\delta \psi} \right), \\
&= \int d^n x d\Gamma \, \frac{\delta F}{\delta m_i} \left[-\psi \frac{\partial}{\partial x^i} \left(\frac{\delta G}{\delta \psi} \right) - \sum_{a=1}^N \mathcal{P}_a \left(y, -\frac{\partial}{\partial x} \right) \cdot \left(\psi \frac{\partial}{\partial y_{(a)}^i} \left(\frac{\delta G}{\delta \psi} \right) \right) \right] \\
&\quad + \int d^n x d\Gamma \, \frac{\delta F}{\delta \psi} \left[-\frac{\partial}{\partial x^i} \left(\frac{\delta G}{\delta m_i} \psi \right) - \sum_{a=1}^N \frac{\partial}{\partial y_{(a)}^i} \left(\left(\mathcal{P}_a \left(y, \frac{\partial}{\partial x} \right) \cdot \frac{\delta G}{\delta m_i} \right) \psi \right) \right]. \tag{6.6}
\end{aligned}$$

We have repeatedly integrated by parts to obtain the terms multiplying to $\delta F/\delta m_i$ and $\delta F/\delta \psi$, using the fact that \mathcal{P}_a is a polynomial of degree a in $\partial/\partial x$. Given a Hamiltonian functional H , we find that the extra body force on the fluid \mathcal{F}_i and the time evolution of the distribution function ψ are given by

$$\mathcal{F}_i = \int d\Gamma \left[-\psi \frac{\partial}{\partial x^i} \left(\frac{\delta H}{\delta \psi} \right) - \sum_{a=1}^N \mathcal{P}_a \left(y, -\frac{\partial}{\partial x} \right) \cdot \left(\psi \frac{\partial}{\partial y_{(a)}^i} \left(\frac{\delta H}{\delta \psi} \right) \right) \right], \tag{6.7}$$

$$\dot{\psi} = -\frac{\partial}{\partial x^i} \left(\frac{\delta H}{\delta m_i} \psi \right) - \sum_{a=1}^N \frac{\partial}{\partial y_{(a)}^i} \left(\psi \mathcal{P}_a \left(y, \frac{\partial}{\partial x} \right) \cdot \frac{\delta H}{\delta m_i} \right). \tag{6.8}$$

6.1 Conservation of fluid momentum for the multibead-chain models

We specialise to Hamiltonians of the form

$$H[\mathbf{m}, \rho, \psi] = H_{fluids}[\mathbf{m}, \rho] + H_s[\psi], \quad H_s[\psi] = \int d^n x d\Gamma (E(y)\psi + k_B T \psi \log \psi), \tag{6.9}$$

where $E(y)$ is some function of the variables $y_{(1)}, \dots, y_{(N)}$. The force on the fluid is given by (6.7) as

$$\mathcal{F}_i = -(N+1)k_B T \frac{\partial}{\partial x^i} \left(\int d\Gamma \, \psi \right) - \int d\Gamma \sum_{a=1}^N \mathcal{P}_a \left(y, -\frac{\partial}{\partial x} \right) \cdot \left(\psi \frac{\partial E}{\partial y_{(a)}^i} \right). \tag{6.10}$$

For each a , the polynomial $\mathcal{P}_a(y, -\partial/\partial x)$ can be written as

$$\mathcal{P}_a \left(y, -\frac{\partial}{\partial x} \right) = \mathcal{Q}_a^j \left(y, -\frac{\partial}{\partial x} \right) \left(-\frac{\partial}{\partial x^j} \right) = -y_{(a)}^j \frac{\partial}{\partial x^j} + O \left(\frac{\partial^2}{\partial x^2} \right), \tag{6.11}$$

where $\mathcal{Q}_a^j(y, -\partial/\partial x)$ is some other polynomial. This is a direct consequence of property (ii) for the polynomials $\mathcal{P}_a(y, -\partial/\partial x)$. The important point here is that $\mathcal{Q}_a^j(y, -\partial/\partial x) = y_{(a)}^j + O(\partial/\partial x)$, meaning that the only term in the operator $\mathcal{Q}_a^j(y, -\partial/\partial x)$ that does not take x -derivatives of its argument is $y_{(a)}^j$.

We can thus write the force as the divergence of a stress tensor, $\mathcal{F}_i = \partial \sigma_i^j / \partial x^j$, for

$$\sigma_i^j = -(N+1)k_B T \delta_i^j \int d\Gamma \, \psi + \int d\Gamma \sum_{a=1}^N \mathcal{Q}_a^j \left(y, -\frac{\partial}{\partial x} \right) \cdot \left(\psi \frac{\partial E}{\partial y_{(a)}^i} \right). \tag{6.12}$$

In particular, if $E(y)$ is a *polynomial* in $y_{(1)}, \dots, y_{(N)}$, then σ_i^j depends on a finite number of *polynomial moments* of ψ and their x -derivatives.

The fact that the force is the divergence of a stress tensor implies the conservation of fluid linear momentum. For certain forms of the energy per chain $E(y)$, we can show that the antisymmetric part of the stress tensor is the divergence of a 3-index tensor, a condition that is sufficient to guarantee conservation of fluid angular momentum.

For example, suppose $E(y)$ depends on the variables $y_{(a)}^i$ only through their *squares* $s_{(a)} = (1/2)\delta_{ij}y_{(a)}^i y_{(a)}^j$, so that

$$E(y) = E(s_{(1)}, \dots, s_{(N)}). \tag{6.13}$$

As $\partial E / \partial y_{(a)}^i = \delta_{ik} y_{(a)}^k \partial E / \partial s_{(a)}$, the stress tensor $\sigma^{jk} = \sigma_i^j \delta^{ik}$ can be written as

$$\sigma^{jk} = -(N+1)k_B T \delta^{jk} \left(\int d\Gamma \psi \right) + \sum_{a=1}^N \left(\int d\Gamma y_{(a)}^j y_{(a)}^k \frac{\partial E}{\partial s_{(a)}} \psi \right) + \frac{\partial}{\partial x^i} T^{jlk}, \quad (6.14)$$

where the tensor T^{jlk} depends on ψ and the explicit form of E . This automatically guarantees that the antisymmetric part of the stress tensor is an exact divergence, i.e. can be considered as an angular momentum flux $A^{jlk} = T^{jlk} - T^{klj}$. In terms of generalised continuum systems, this term has a similar interpretation to the asymmetric stress for the 3-bead chain suspensions considered in section 5.1, as a term that is balanced by the divergence of a couple stress.

6.2 Closure of the multibead-chain models without dissipation

Having investigated the force term in (6.7) and the relationship between the energy and the conservation laws in section 6.1, we proceed to investigate the evolution equation (6.8) for ψ in the multibead-chain model without dissipation. If $E(y)$ is a polynomial in $y_{(1)}, \dots, y_{(N)}$, then as we have seen in the last section, the stress tensor depends on a finite number of polynomial moments of ψ . We will show that, in this system, we can achieve closure with a finite set of polynomial moments.

Recall that that \mathcal{P}_a is homogeneous with order a as a polynomial in y with coefficients in $\partial/\partial x$, by property (iii). Given a polynomial $p(y)$ which is homogeneous of order b , consider the time evolution of the corresponding polynomial moment $\langle p(y) \rangle = \int d\Gamma p(y) \psi$, where as before angle brackets denote integration over all y -space against ψ . This is explicitly given by

$$\begin{aligned} \langle \dot{p}(y) \rangle &= -\frac{\partial}{\partial x^i} (u^i(x) \langle p(y) \rangle) - \sum_{a=1}^N \int d\Gamma p(y) \frac{\partial}{\partial y_{(a)}^i} \left(\psi \mathcal{P}_a \left(y, \frac{\partial}{\partial x} \right) \cdot u^i(x) \right), \\ &= -\frac{\partial}{\partial x^i} (u^i(x) \langle p(y) \rangle) + \sum_{a=1}^N \left\langle \frac{\partial p(y)}{\partial y_{(a)}^i} \mathcal{P}_a \left(y, \frac{\partial}{\partial x} \right) \right\rangle \cdot u^i(x), \end{aligned} \quad (6.15)$$

where the factors of $\partial/\partial x$ in \mathcal{P}_a act on u^i (and not on ψ). If $p(y)$ is homogeneous with order b , then $\partial p(y)/\partial y_{(a)}^i$ is either identically zero, or a homogeneous polynomial of order $b-a$. Therefore

$$\frac{\partial p(y)}{\partial y_{(a)}^i} \mathcal{P}_a \left(y, \frac{\partial}{\partial x} \right) \cdot u^i(x)$$

is a homogeneous polynomial in y with order b , with coefficients in $u^i(x)$ and its spatial derivatives.

We deduce that given the flow field $u^i(x)$, the collection of homogeneous polynomials of order b form a closed system for each b . If in addition, $E(y)$ is a polynomial in $y_{(1)}, \dots, y_{(N)}$, then the stress tensor depends on a finite number of polynomial moments of ψ (and their x -derivatives). If the highest order of the polynomials that appear in the expression of the stress tensor is b_{max} , we can achieve a finite closure by collect up the evolution equations for all monomial moments with order at most b_{max} .

A closure can still be achieved if the time evolution of higher order polynomial moments depends on both equal and lower order polynomial moments; but if the time evolution of lower order polynomial moments depend on higher order polynomial moments, then an exact, finite closure is impossible in general. We will return to this point when we consider the multibead-chain model with dissipation.

6.3 The multibead-chain models with dissipation

Now we consider the multibead-chain model with a dissipation bracket. Consider the Riemannian metric g on the configuration space of the multibead chain, with line element written as

$$ds^2 = \delta_{ij} dx^i dx^j + \sum_{a=1}^N \delta_{ij} dy_{(a)}^i dy_{(a)}^j, \quad (6.16)$$

and let \tilde{g} denote the inverse of g . (See appendix B for a discussion for generalisations to arbitrary Riemannian manifolds.) We define a dissipation bracket on functionals F, G by

$$\begin{aligned} (F, G) &= \int d^n x d\Gamma \psi \tilde{g} \left(d \left(\frac{\delta F}{\delta \psi} \right), d \left(\frac{\delta G}{\delta \psi} \right) \right), \\ &= \int d^n x d\Gamma \psi \left[\delta^{ij} \frac{\partial}{\partial x^i} \left(\frac{\delta F}{\delta \psi} \right) \frac{\partial}{\partial x^j} \left(\frac{\delta G}{\delta \psi} \right) + \sum_{a=1}^N \delta^{ij} \frac{\partial}{\partial y_{(a)}^i} \left(\frac{\delta F}{\delta \psi} \right) \frac{\partial}{\partial y_{(a)}^j} \left(\frac{\delta G}{\delta \psi} \right) \right]. \end{aligned} \quad (6.17)$$

Given a Hamiltonian functional H , which should now be interpreted as the free energy, the time evolution of a functional F is given by

$$\dot{F} = \{F, H\} - \frac{1}{\zeta}(F, H) \quad (6.18)$$

for some parameter $\zeta > 0$. This implements a linear mobility relation with mobility $1/\zeta$. The expression for the stress tensor in terms of the functional derivatives of H is not altered by this dissipation bracket. However, the time evolution of ψ will be altered, which in turn affects the closure properties of the system.

Consider free energies of the form (6.9), and further specialise to energy functions $E(y)$ that are *quadratic* in each internal degree of freedom, i.e.

$$E(y) = \sum_{a=1}^N \frac{\kappa_a}{2} \delta_{ij} y_{(a)}^i y_{(a)}^j, \quad (6.19)$$

where $\kappa_a > 0$ are parameters that describe the stiffness of each normal mode. This energy function produces a stress that conserves angular momentum, as seen in section 6.2. The evolution equation for ψ is then

$$\dot{\psi} + \frac{\partial}{\partial x^i} (u^i(x) \psi) + \sum_{a=1}^N \frac{\partial}{\partial y_{(a)}^i} \left(\psi \mathcal{P}_a \left(y, \frac{\partial}{\partial x} \right) \cdot u^i(x) \right) = \frac{k_B T}{\zeta} \nabla_x^2 \psi + \sum_{a=1}^N \left(\frac{\kappa_a}{\zeta} \frac{\partial}{\partial y_{(a)}^i} \left(y_{(a)}^i \psi \right) + \frac{k_B T}{\zeta} \nabla_{y_{(a)}}^2 \psi \right), \quad (6.20)$$

where $\nabla_x^2 = \delta^{ij} \partial^2 / \partial x^i \partial x^j$, and $\nabla_{y_{(a)}}^2 = \delta^{ij} \partial^2 / \partial y_{(a)}^i \partial y_{(a)}^j$ for $a = 1, \dots, N$. The terms due to the dissipation bracket have been collected to the right-hand side. These new terms can be interpreted as the drift terms and the diffusive terms in a *Fokker-Planck equation*. The drift terms can be attributed to the internal energy term in the free energy H_s , while the diffusive terms can be attributed to the entropy term in H_s .

For this specific form of the energy, the time evolution of a polynomial moment $\langle p(y) \rangle$ of order b depends on polynomial moments of order b or lower. This is directly verified by integrating by parts – the drift terms do not alter the order (or gives zero), while the diffusion terms always lower the order. So the multibead-chain model with linear dissipation has a finite closure for quadratic energy.

We find an explicit expression for the stress tensor using (6.12, 6.14):

$$\begin{aligned} \sigma^{jk} &= - (N+1) k_B T \delta^{jk} \int d\Gamma \psi + \sum_{a=1}^N \int d\Gamma \kappa_a y_{(a)}^k \mathcal{Q}_a^j \left(y, -\frac{\partial}{\partial x} \right) \cdot \psi, \\ &= - (N+1) k_B T \delta^{jk} \int d\Gamma \psi + \sum_{a=1}^N \int d\Gamma \kappa_a y_{(a)}^j y_{(a)}^k \psi + \frac{\partial}{\partial x^l} \left(\sum_{a=1}^N \int d\Gamma y_{(a)}^k \mathcal{R}_a^{jl} \left(y, -\frac{\partial}{\partial x} \right) \cdot \psi \right), \end{aligned} \quad (6.21)$$

where \mathcal{R}_a^{jl} is defined in terms of \mathcal{P}_a and \mathcal{Q}_a^j by

$$\mathcal{P}_a \left(y, -\frac{\partial}{\partial x} \right) = \mathcal{Q}_a^j \left(y, -\frac{\partial}{\partial x} \right) \left(-\frac{\partial}{\partial x^j} \right) = -y_{(a)}^j \frac{\partial}{\partial x^j} + \mathcal{R}_a^{jl} \left(y, -\frac{\partial}{\partial x} \right) \frac{\partial^2}{\partial x^j \partial x^l}. \quad (6.22)$$

The quantity \mathcal{R}_a^{jl} is a polynomial in y with coefficients in $\partial/\partial x$. It is identically zero for $a = 1$, and a nonzero homogeneous polynomial of order a for $a \geq 2$. So the order of the polynomial moments needed to describe the stress tensor σ^{jk} in (6.21) does not exceed $2N$.

The hydrodynamic terms, the drift terms and the x -diffusion term in the evolution equation (6.20) for ψ only couples monomial moments of order b to monomial moments of the same order, while the $y_{(a)}$ -diffusion term couples monomial moments of order b to monomial moments of order $b - 2a$ (or gives 0). So it is sufficient to consider the even order monomial moments up to order $2N$. This is consistent with the Hookean 3-bead chain considered in section 5.2, where the monomial moments required are precisely those of orders 0, 2 and 4.

A slightly more general sufficient condition on $E(y)$ for finite closure to be possible is that

$$\text{for all } a = 1, \dots, N, \quad \frac{\partial E}{\partial y_{(a)}^j} \text{ is a polynomial in } y \text{ of order less than or equal to } a. \quad (6.23)$$

This property is evidently satisfied for quadratic energies. We call a polynomial $p(y)$ satisfying property (6.23) *admissible*, and other polynomials *inadmissible*. An admissible $E(y)$ leads to a finite closure because the drift term in the evolution equation for ψ due to internal relaxation is

$$\frac{1}{\zeta} \sum_{a=1}^N \frac{\partial}{\partial y_{(a)}^i} \left(\delta^{ij} \frac{\partial E}{\partial y_{(a)}^j} \psi \right).$$

The hydrodynamic and diffusion terms only couple polynomial moments to other moments of equal or lower order. When $E(y)$ is admissible, the expression above suggests that the drift terms only couple moments to other moments of equal or lower order. Thus an *order-counting* argument can be used to find an exact, finite closure.

Since we are only considering internal energies $E(y)$ that are polynomials, the stress tensor can be described by a finite number of moments. If the maximum order of the required moments is b_{max} and $E(y)$ is admissible, collecting all monomials of order less than or equal to b_{max} results in a closed system. The argument is the same as that used to demonstrate finite closure for quadratic energies of the form (6.19).

While $E(y)$ being admissible is nominally more general than $E(y)$ being of the Hookean-like form (6.19), we have the following highly constraining result:

Proposition. $E(y)$ is admissible (in the sense of (6.23)) if and only if

$$E(y) = \sum_{a=1}^N \left(\lambda_{(a)i} y_{(a)}^i + \frac{1}{2} \kappa_{(a)ij} y_{(a)}^i y_{(a)}^j \right) + C,$$

where $C, \lambda_{(a)i}, \kappa_{(a)ij}$ are constants, with $\kappa_{(a)ij} = \kappa_{(a)ji}$.

Proof. Suppose $p(y)$ is inadmissible, and $q(y)$ is an arbitrary polynomial that is not identically zero. We claim that p being inadmissible implies that pq is inadmissible. Suppose that

$$\frac{\partial p}{\partial y_{(a)}^j} \text{ has order strictly greater than } a, \text{ for some } a.$$

Then

$$\frac{\partial}{\partial y_{(a)}^j} (pq) = \frac{\partial p}{\partial y_{(a)}^j} q + p \frac{\partial q}{\partial y_{(a)}^j}$$

has order strictly greater than a , since q is not identically zero, and $\partial p / \partial y_{(a)}^j$ has order strictly greater than a .

We use this to show that all polynomials containing cross terms are inadmissible by showing that the “lowest” cross term is inadmissible. If $p(y) = \tau_{ij} y_{(a)}^i y_{(b)}^j$ for $a \neq b$, where τ_{ij} are constants that are not identically zero, then without loss of generality we can assume $a < b$, and thus

$$\frac{\partial}{\partial y_{(a)}^k} \left(\tau_{ij} y_{(a)}^i y_{(b)}^j \right) = \tau_{kj} y_{(b)}^j \text{ has order } b > a,$$

so this $p(y)$ is inadmissible. Therefore if $E(y)$ is admissible, it cannot contain any cross terms, and hence can be written in the form

$$E(y_{(1)}, \dots, y_{(N)}) = \sum_{a=1}^N E_a(y_{(a)})$$

for polynomials $E_a(y_{(a)})$. Now admissibility is equivalent to

$$\frac{\partial E(y)}{\partial y_{(a)}^j} = \frac{\partial E_a(y_{(a)})}{\partial y_{(a)}^j} \text{ has order less than or equal to } a \text{ for all } a = 1, \dots, N.$$

This is equivalent to E_a being linear-quadratic in $y_{(a)}$. The constants of integration for each E_a can be collected together into a single constant C . \square

In particular, among all the admissible (in the sense of (6.23)) choices of energy functions $E(y)$, only the Hookean-like energy functions considered in (6.19) are rotationally invariant. Many physically plausible energy functions, such as that for a non-Hookean bead-spring pair, are not admissible. For such choices, we cannot achieve an exact, finite closure by an order-counting argument in the multibead-chain model with dissipation. Unless a new argument is found, we can only hope to find some reasonable approximations that would give *approximate closure* in these cases, similar to the *Peterlin approximation* for a bead-spring pair with a non-Hookean spring [3, 28].

7 Conclusion

The main focus of this paper is on the formulation and analysis of models for multibead-chain suspensions in an ideal fluid. We have modelled the suspension as a double bracket system, with a Hamiltonian part described by a noncanonical Poisson bracket, and a dissipation bracket to account for resistive and diffusive effects.

The resulting system describes the coupling of ideal compressible hydrodynamics to the distribution function $\psi(x, y)$ of multibead-chains in configuration space, where x and y are the macroscopic and internal degrees of freedom respectively. This description is valid when the macroscopic lengthscales are sufficiently large, and the microscopic lengthscales of the individual chains are sufficiently small, so that the chains are advected by a Stokes flow while the Newtonian viscous stress on the fluid is negligible. If the fluid domain is a manifold M , then the appropriate configuration space for an $(N + 1)$ -bead chain is the N^{th} order tangent bundle $T^{(N)}M$. The Hamiltonian part of the system, which consists of the advection of the beads in the multibead-chain by the fluid as Lagrangian markers, can be described by a Poisson bracket, which has been constructed using the machinery of the semidirect product Lie–Poisson formulation. The dissipative part of the system, consisting of the effects of internal relaxation and Brownian diffusion, can be effectively captured by a metric dissipation bracket. For suitable choices of the free energy, the non-Hamiltonian terms can be considered as a Fokker–Planck diffusion operator on the distribution function $\psi(x, y)$.

One of the main advantages for such a double bracket formulation is that, given a Hamiltonian functional (or free energy) that can be written in the form $H = H_{fluids}[\mathbf{m}, \rho] + H_s[\psi]$, where H_{fluids} is the usual ideal fluid Hamiltonian, the elastic body force exerted by the chains on the fluid depends on $\delta H / \delta \psi$ only and can be calculated from a direct manipulation of the Poisson bracket. We have obtained explicit expressions for the particle-contributed stress tensor for a wide range of free energies in the multibead-chain model with this method. We found that the stress tensor is generically asymmetric, but nonetheless for reasonable choices of the internal energy $E(y)$, the antisymmetric part of the stress tensor can be written as the divergence of a 3-index tensor, which we interpret as an angular momentum flux, as in [4, 5]. This effect is absent in the bead-spring pair models, and any model that assumes a linear flow around the multibead-chain is in fact equivalent to modelling a number of bead-spring pairs with a common centre.

A major concern in using a distribution function description for the multibead-chains is that the evolution equation of $\psi(x, y)$ involves both the macroscopic (x) and internal (y) degrees of freedom. In other words, it is a partial differential equation in a large number of dimensions, which is computationally expensive to solve. However, the particle-contributed stress typically depends only on some statistical properties of the internal degrees of freedom, i.e. some y -integrals of the distribution function $\psi(x, y)$. Therefore it is desirable to find a finite set of these y -integrals, such that:

1. The stress tensor is completely described by these y -integrals.
2. These y -integrals form a closed system of evolution equations, given the fluid velocity field $\mathbf{u}(x, t)$ and its spatial derivatives.

When this is possible, we can model the multibead-chain suspension by evolving a number of macroscopic fields (depending on x only), instead of having to consider both the macroscopic (x) and internal (y) degrees of freedom. We have shown that, if we choose a certain quadratic form for the internal energy $E(y)$, such a finite closure is possible for an arbitrary multibead-chain. These can be considered as analogues of the upper-convected Maxwell model for bead-spring pairs.

Within the framework of the distribution function approach, exact closure is a rare property that is only satisfied for rather restrictive choices of the internal energy. For other choices of the internal energy, we have to evolve the full distribution $\psi(x, y)$, which is much more computationally expensive than evolving x -dependent fields. The closure problem is clearly visible in the bead-spring pair model for non-Hookean springs, and our work heavily suggests that an entirely analogous obstacle exists for multibead-chain models.

A parallel line of development, which resolves this particular problem, would be to start with *internal state variables*, which are phenomenological x -dependent fields that are assumed to completely characterise the internal structure of the complex fluids. This means that the macroscopic fluid properties such as the particle-contributed stress are postulated to be completely determined by the chosen internal state variables. Mathematically, these internal state variables are typically sections of some naturally constructed fibre bundles, e.g. tensor fields. The hydrodynamic part of the evolution of such variables is then captured by an appropriate material derivative along the fluid velocity field. For example, if the conformation tensor $C^{jk}(x)$ is chosen to be the internal state variable, the appropriate material derivative would be the familiar *upper-convected derivative*, or for more general tensor fields the *Lie derivative*. Analogous semidirect product Lie–Poisson structures exist for such a description, and have been extensively studied in [20, 21], with various applications to complex fluids [1, 2, 9, 12, 13, 19] and to magnetohydrodynamics [20, 27].

However, the internal state variable description has a different problem – the equations are easy to solve, but difficult to write down. Not only is it difficult to connect the postulated form of the free energy to a microscopic toy model of the suspended bodies, the imposition of the mobility relations has also become much more arbitrary. Unlike in the distribution function approach, there is no obvious way to convert a microscopic toy model for the suspended bodies to the relaxation and dissipation terms for the internal state variables. In other words, the appropriate form of the dissipation bracket has to be guessed. The form of dissipation bracket can be constrained by requiring material invariance and the satisfaction of thermodynamic principles, which

rules out some choices as unphysical, but this does not fundamentally eliminate the arbitrariness of such a choice. Another perhaps more glaring source of arbitrariness is the choice of the internal state variables – how many of them do we assume to be sufficient to describe the internal state phenomenologically?

Conversely, in the distribution function approach, the evolution equations for the distribution function are easy to write down but difficult to solve. The microphysics of the suspended body is directly implemented into the evolution equation of the distribution function $\psi(x, y)$, which gives a complete ensemble description of the suspended bodies. The internal relaxation force is simply a gradient of the internal energy, and the diffusive Brownian force can be expediently captured in terms of the Boltzmann entropy of the distribution function $\psi(x, y)$ [12]. The mobility relation is in principle determined by the internal structure of the suspended body, although we have only worked with linear approximations. The resulting equation has a clear physical interpretation as a Fokker–Planck equation, consisting of the hydrodynamic drift, internal relaxation and Brownian diffusion of the distribution function $\psi(x, y)$. There is no room for arbitrariness – once the internal microphysics of the suspended body is determined, we can immediately write down the governing equations for the fluid suspension based on this information. Moreover, when an exact closure is possible, the distribution function approach reduces to the internal state variable approach exactly, as far as the macroscopic behaviour of the fluid suspension is concerned. This process also selects the appropriate internal state variables that are necessary for a complete macroscopic description of the suspension.

Having made the case for the complementary nature of the two approaches, we note however that the distribution function approach has been largely abandoned since [12, 13]. We hope that this paper will revive the interest in modelling fluid suspensions with distribution functions, in particular as part of a *combined approach*, where one uses the distribution function as a starting point to implement the microphysics of the suspended bodies, then proceed to make approximations to obtain effective equations in terms of internal state variables. This approach is largely unexplored beyond the bead-spring pair models, and we believe that it informs the phenomenological approach based on internal state variables.

Acknowledgements

The author wishes to thank Paul Dellar for bringing to our attention the connection between the asymmetric stress tensors encountered in the multibead-chain suspensions and the couple stresses in a generalised continuum system, among his numerous comments and suggestions. This work was supported by the Mathematical Institute, University of Oxford, which played no other role in the research, or in the preparation and submission of the manuscript.

A Proof sketch for the homomorphism property of complete lifts to $T^{(N)}M$

In this appendix we sketch a proof for the homomorphism property of complete lifts of vector fields $\mathbf{u} \in \text{Vect}(M)$ to $\mathbf{u}^\# \in \text{Vect}(T^{(N)}M)$ (3.10, 4.8). For more details, see [34].

Let M be a manifold. Define a *diffeomorphism* $\varphi : M \rightarrow M$ to be a smooth bijective map from M to M with a smooth inverse. In the language of tensor calculus, a diffeomorphism φ can be thought of as a coordinate transformation $x^i \mapsto \varphi^i(x)$. The collection of diffeomorphisms of a manifold M is denoted by $\text{Diff}(M)$, which can be thought of as an infinite-dimensional Lie group [8, 17].

Let φ, ψ be diffeomorphisms from M to itself. Consider a path $\alpha : I \rightarrow M$, where I is some closed interval containing 0 in its interior. Then the diffeomorphism φ can act on paths $\alpha(t)$ by

$$\varphi^\# : \alpha(t) \mapsto (\varphi \circ \alpha)(t). \quad (\text{A.1})$$

Since the composition of functions is associative, this action satisfies the homomorphism property:

$$(\varphi \circ \psi)^\# (\alpha) = \varphi^\# (\psi^\# (\alpha)) = (\varphi \circ \psi \circ \alpha)(t). \quad (\text{A.2})$$

Now consider equivalence classes of paths under the equivalence relation $\overset{(N)}{\sim}$ defined by

$$\alpha(t) \overset{(N)}{\sim} \beta(t) \Leftrightarrow \alpha(0) = \beta(0), \left. \frac{d^a}{dt^a} \alpha(t) \right|_{t=0} = \left. \frac{d^a}{dt^a} \beta(t) \right|_{t=0} \text{ for } a = 1, \dots, N. \quad (\text{A.3})$$

The equivalence relation $\overset{(N)}{\sim}$ identifies paths that have the same Taylor series up to order N at $t = 0$. Now suppose we have a path $\alpha(t)$ with coordinate expression

$$\alpha^i(t) = x^i + \sum_{a=1}^N y_{(a)}^i \frac{t^a}{a!} + O(t^{N+1}). \quad (\text{A.4})$$

If $\varphi^i(x)$ is the coordinate expression for φ , then comparing powers of t gives coordinates of the path $(\varphi^\#(\alpha))(t)$ as

$$(\varphi^\#(\alpha))^i(t) = \varphi^i(\alpha(t)) = \varphi^i(\alpha(0)) + \sum_{a=1}^N \frac{t^a}{a!} \left(\frac{d^a}{dt^a} \varphi^i(\alpha(t)) \right) \Big|_{t=0} + O(t^{N+1}). \quad (\text{A.5})$$

Note that

$$\frac{d^a}{dt^a} \varphi^i \left(x^i + \sum_{a=1}^N y_{(a)}^i \frac{t^a}{a!} + O(t^{N+1}) \right) \Big|_{t=0} \quad (\text{A.6})$$

does not depend on the $O(t^{N+1})$ terms when $a \leq N$. So $\varphi^\#$ descends to a well-defined map on equivalence classes of paths under $\stackrel{(N)}{\sim}$, i.e. equivalence classes of paths with the same Taylor series at $t = 0$ up to order N . We also denote this map by $\varphi^\#$. Thus we have obtained an association

$$\varphi \in \text{Diff}(M) \mapsto \varphi^\# \in \text{Diff}(T^{(N)}M), \quad (\text{A.7})$$

such that $(\varphi \circ \psi)^\# = \varphi^\# \circ \psi^\#$, i.e. it is a *group homomorphism*. By differentiating this correspondence, i.e. by writing

$$\varphi^i(x) = x^i + su^i(x) + O(s^2), \quad (\text{A.8})$$

$$\psi^i(x) = x^i + rv^i(x) + O(r^2), \quad (\text{A.9})$$

and comparing the two sides of the expression

$$\frac{\partial^2}{\partial s \partial r} \Big|_{s=0, r=0} (\varphi \circ \psi \circ \varphi^{-1})^\# = \frac{\partial^2}{\partial s \partial r} \Big|_{s=0, r=0} (\varphi^\# \circ \psi^\# \circ (\varphi^{-1})^\#), \quad (\text{A.10})$$

we obtain a homomorphism of Lie algebras

$$\mathbf{u} \in \text{Vect}(M) \mapsto \mathbf{u}^\# \in \text{Vect}(T^{(N)}M), \quad (\text{A.11})$$

which is precisely the complete lift given in (4.8).

B Vector bundle structure and metrics on $T^{(N)}M$

This appendix addresses the geometric interpretation of some of the expressions we have encountered. We will assume some familiarity with vector bundles and Riemannian geometry. Detailed expositions can be found in [16, 32].

B.1 Vector bundle structure on $T^{(N)}M$

Let $T^{(N)}M$ be the N^{th} order tangent bundle of the manifold M . As before, if x^i is a coordinate system on M , it induces a coordinate system $(x^i, y_{(a)}^i)$ on $T^{(N)}M$, where the fibre coordinates $y_{(a)}^i$, $a = 1, \dots, N$ denote the a^{th} derivatives of the equivalence class of paths attached to x .

Given a coordinate transformation $x^i \mapsto \tilde{x}^i$, the induced coordinate transformation $(x^i, y_{(a)}^i) \mapsto (\tilde{x}^i, \tilde{y}_{(a)}^i)$ is not linear for $a \geq 2$. For example,

$$\tilde{y}_{(2)}^i = \frac{\partial \tilde{x}^i}{\partial x^j} y_{(2)}^j + \frac{\partial^2 \tilde{x}^i}{\partial x^j \partial x^k} y_{(1)}^j y_{(1)}^k. \quad (\text{B.1})$$

(See appendix A.) In particular, the fibre coordinates do not transform like vectors under an arbitrary coordinate transformation.

In previous sections we have considered moments of the distribution function of the form

$$\int d\Gamma y_{(a)}^i \psi(x, y) \quad \text{for } a \geq 2 \text{ (say)}, \quad (\text{B.2})$$

where $d\Gamma = d^n y_{(1)} \cdots d^n y_{(N)}$ as before. Since the fibre coordinates do not transform linearly, we cannot not make invariant sense of linear operations on the fibre coordinates, such as sums and integrals. In more geometric terms, the transition maps between two overlapping charts $(x^i, y_{(a)}^i) \mapsto (\tilde{x}^i, \tilde{y}_{(a)}^i)$ of $T^{(N)}M$ are not linear in the fibre coordinates for $N \geq 2$. These charts therefore do not give $T^{(N)}M$ the *structure of a vector bundle*.

However, we can produce an isomorphism from $T^{(N)}M$ to $(T \oplus \dots \oplus T)M$ (N times) with the help of a *metric*, or more generally a *connection* on the tangent bundle [6, 7]. Given a metric g on M , we can consider its *Riemannian connection* ∇ (also known as the *Levi-Civita connection*), which (roughly speaking) defines the infinitesimal parallel transport of vector field $Y = Y^i \partial / \partial x^i$ along vector field $X = X^i \partial / \partial x^i$ to be $\nabla_X Y$, given in coordinates by

$$\nabla_X Y = X^j \left(\frac{\partial Y^i}{\partial x^j} + \Gamma_{jk}^i Y^k \right) \frac{\partial}{\partial x^i}, \quad (\text{B.3})$$

where Γ_{jk}^i are the usual *Christoffel symbols* of the connection, defined by

$$\nabla_{\frac{\partial}{\partial x^j}} \frac{\partial}{\partial x^k} = \Gamma_{jk}^i \frac{\partial}{\partial x^i}. \quad (\text{B.4})$$

The following construction works for any connection on TM . General connections are considered in appendix **B.2**. Let $\alpha(t)$ be a curve on M , with $v(t) = d\alpha(t)/dt$ its velocity vector at time t , which is a vector field along the curve $\alpha(t)$. If $w(t)$ is another vector field along the curve $\alpha(t)$, we can define its *covariant derivative*, conventionally written as Dw/dt , along the curve $\alpha(t)$ as follows. If $W(x)$ is a vector field on M , such that $W(\alpha(t)) = w(t)$, i.e. W agrees with w along the curve $\alpha(t)$, then we define

$$\frac{Dw}{dt}(t) = \nabla_{v(t)} W(\alpha(t)). \quad (\text{B.5})$$

Applying the chain rule $(\partial W^i / \partial x^j)(\partial \alpha^j / \partial t) = \partial w^i / \partial t$ gives the following coordinate expression for the covariant derivative:

$$\left(\frac{Dw}{dt} \right)^i = \frac{\partial w^i}{\partial t} + \Gamma_{jk}^i v^j(t) w^k(t). \quad (\text{B.6})$$

The components $(Dw/dt)^i$ transform like a vector under a change of coordinates, as long as the Christoffel symbols Γ_{jk}^i are transformed appropriately.

In particular, we can apply the covariant derivative D/dt iteratively on the velocity vector field $v(t) = d\alpha(t)/dt$ along the curve $\alpha(t)$ to obtain the *covariant acceleration* Dv/dt and higher order covariant derivatives. We show that we can write the first N coordinate derivatives of the path α at $t = 0$ in terms of the covariant derivatives $v(0), Dv/dt(0), \dots, (D^{N-1}v/dt^{N-1})(0)$ evaluated at $t = 0$, which are genuine tangent vectors at $\alpha(0)$. This produces an isomorphism from $T^{(N)}M$ to $(T \oplus \dots \oplus T)M$ (N times), and the latter is a vector bundle by construction. We describe this isomorphism explicitly as follows. Let $\alpha(t)$ be a path, with coordinates

$$\alpha^i(t) = x^i + \sum_{a=1}^N y_{(a)}^i \frac{t^a}{a!} + O(t^{N+1}).$$

Its velocity vector field $v(t) = d\alpha(t)/dt$ has coordinates

$$v^i(t) = y_{(1)}^i + \sum_{a=1}^{N-1} y_{(a)}^i \frac{t^a}{a!} + O(t^N). \quad (\text{B.7})$$

Then by iteratively applying D/dt on $v(t)$, we have:

$$\begin{aligned} v(0)^i &= y_{(1)}^i, \\ \left(\frac{Dv}{dt}(0) \right)^i &= y_{(2)}^i + \Gamma_{jk}^i y_{(1)}^j y_{(1)}^k, \\ \left(\frac{D^2 v}{dt^2}(0) \right)^i &= y_{(3)}^i + \Gamma_{jk}^i y_{(1)}^j \left(y_{(2)}^k + \Gamma_{lm}^k y_{(1)}^l y_{(1)}^m \right), \\ &\vdots \\ \left(\frac{D^{N-1} v}{dt^{N-1}}(0) \right)^i &= y_{(N)}^i + \Gamma_{jk}^i y_{(1)}^j \left(\frac{D^{N-2} v}{dt^{N-2}}(0) \right)^k. \end{aligned} \quad (\text{B.8})$$

The Jacobian matrix of the coordinate transformation

$$(x^i, y_{(1)}^i, y_{(2)}^i, \dots, y_{(N)}^i) \mapsto \left(x^i, v(0)^i, \left(\frac{Dv}{dt}(0) \right)^i, \left(\frac{D^2 v}{dt^2}(0) \right)^i, \dots, \left(\frac{D^{N-1} v}{dt^{N-1}}(0) \right)^i \right) \quad (\text{B.9})$$

is upper triangular, with blocks of the identity matrix δ_j^i on the diagonal, so in particular it is invertible and has determinant 1.

Since each of the $(D^a v / dt^a(0))^i$ transform as a tangent (or contravariant) vector, we have produced an isomorphism from $T^{(N)}M$ to $(T \oplus \cdots \oplus T)M$ (N times). Thus the expressions for y -moments of $\psi(x, y)$, such as those in (B.2), can be reinterpreted invariantly using this isomorphism. In more detail:

1. Perform the coordinate transformation (B.9) on all expressions. Geometrically, this is the isomorphism $T^{(N)}M \simeq (T \oplus \cdots \oplus T)M$, so functions, vector fields, differential forms etc. on $T^{(N)}M$ can be transformed correspondingly to those on $(T \oplus \cdots \oplus T)M$.
2. In particular, transform $\psi(x, y)d\Gamma$ into a density on $(T \oplus \cdots \oplus T)M$. Since the Jacobian matrix of the coordinate transformation (B.9) has determinant 1, we can transform the distribution function $\psi(x, y)$ like a scalar function.
3. Compute all moments of $\psi(x, v(0), Dv/dt(0), \dots, D^{N-1}v/dt^{N-1}(0))$ in the new set of coordinates. Since each of the $(D^a v / dt^a(0))^i$ transforms as a vector, the new moments can now be interpreted geometrically as tensor fields (more precisely, fields of tensor densities) on M .

If the manifold M is the Euclidean space \mathbb{R}^n with the standard metric δ_{ij} , then the Christoffel symbols Γ_{jk}^i vanish identically in Cartesian coordinates, so explicit coordinate expressions remain unmodified in this case. Nonetheless, the above procedure gives an invariant interpretation of the moments of ψ , which is useful when one wishes to consider non-Cartesian coordinate systems such as cylindrical polar coordinates, or manifolds that are not flat such as the surface of a sphere.

Nonetheless, the isomorphism from $T^{(N)}M$ to $(T \oplus \cdots \oplus T)M$ we have described is *not canonical*, in the sense that it depends on the choice of a *connection* on TM . While there are complete lifts of vector fields to $T^{(N)}M$ and to $(T \oplus \cdots \oplus T)M$ respectively, neither of them depend on the choice of a connection, so their images under the isomorphism $T^{(N)}M \simeq (T \oplus \cdots \oplus T)M$ do not coincide in general.

B.2 Riemannian metrics on the total space of a vector bundle

Let (M, g) be a Riemannian manifold, and let $\pi : E \rightarrow M$ be a vector bundle with a *Riemannian structure* h , which is a smoothly varying, symmetric positive definite bilinear form $h_x : E_x \times E_x \rightarrow \mathbb{R}$ on each of the fibres $E_x = \pi^{-1}(x)$. We sketch a construction of a Riemannian metric on the total space E of the vector bundle, which in some sense is the closest metric to a block diagonal sum of g and h , using a connection ∇ on the vector bundle. The idea is as follows: the connection splits the tangent spaces to the total space E into vertical and horizontal subspaces, and we can use g on the horizontal subspace and h on the vertical subspace as the inner product.

Let q be the *rank* of the vector bundle E , i.e. the dimension of the fibres $E_x = \pi^{-1}(x)$. Denote a point on the vector bundle E by (x, ξ) , where x is a point on M , and $\xi \in E_x$ is a vector. A (*smooth*) *section* of the vector bundle E is a smooth map $\sigma : M \rightarrow E$ such that $\pi \circ \sigma = id_M$ is the identity map on M . We will denote the space of all sections as $\Gamma(E)$.

To set out our notation, we recall a few standard definitions. A *connection* on a vector bundle E is a map $\nabla : \text{Vect}(M) \times \Gamma(E) \rightarrow \Gamma(E)$, which formalises the idea of an infinitesimal parallel transport of a section σ along a vector field X on M , denoted as $\nabla_X \sigma$. It is required to satisfy the following properties:

$$\nabla_{(fX+gY)}\sigma = f\nabla_X\sigma + g\nabla_Y\sigma, \quad (\text{B.10})$$

$$\nabla_X(a\sigma + \tau b) = a\nabla_X\sigma + b\nabla_X\tau, \quad (\text{B.11})$$

$$\nabla_X(f\sigma) = (X \cdot f)\sigma + f\nabla_X\sigma, \quad (\text{B.12})$$

for all smooth functions f, g on M , all vector fields X, Y on M , all real numbers a, b , and all sections σ, τ of E . Condition (B.10) implies that the expression $\nabla\sigma$ can alternatively be interpreted as a section-valued 1-form on M , since it is $C^\infty(M)$ -linear in its first argument. Condition (B.11) implies that the connection is \mathbb{R} -linear in its second argument. Condition (B.12) can be interpreted as a form of the *Leibniz rule* – in terms of section-valued 1-forms, it is equivalent to

$$\nabla(f\sigma) = df \cdot \sigma + f\nabla\sigma, \quad (\text{B.13})$$

where the dot denotes the tensor product over $C^\infty(M)$, which we suppress throughout in our notation. We call $\nabla\sigma$ the *covariant derivative* of the section σ . We can allow connections to act on *local sections* $\sigma : U \rightarrow E|_U = \pi^{-1}(U)$, where U is an open set in M , by restriction. This will be useful in finding local coordinate expressions later.

Let U be a *framed open set* on M , i.e. an open set on M equipped with q local sections $s_\alpha : U \rightarrow E|_U = \pi^{-1}(U)$, $\alpha = 1, \dots, q$ such that $s_1(x), \dots, s_q(x)$ are linearly independent for all x on U . The collection of local

sections s_α is called a *frame*. Framed open sets always exists, since vector bundles are *locally trivial*, i.e. for sufficiently small open sets U of M , there is always an isomorphism $E|_U \simeq U \times \mathbb{R}^q$, and the choice of frame is equivalent to a choice of such an isomorphism. This is also called a *local trivialisation* of the vector bundle.

Thus, a choice of frame s_α endows $E|_U = \pi^{-1}(U)$ with a coordinate system. In more detail, any point in $E|_U$ can be described by $\dim(M) + q$ coordinates (x^i, ξ^α) , where

$$(x, \xi) = (x^i, \xi^\alpha s_\alpha). \quad (\text{B.14})$$

If ∇ is a connection on the vector bundle E , its local expression relative to the frame $s_1(x), \dots, s_q(x)$ can be given in terms of the *connection matrix* ω_α^β as

$$\nabla s_\alpha = \omega_\alpha^\beta s_\beta = \omega_{i\alpha}^\beta(x) dx^i s_\beta, \quad (\text{B.15})$$

where $\omega_\alpha^\beta = \omega_{i\alpha}^\beta(x) dx^i$ should be interpreted as a matrix of 1-forms on U . For example, if $E = TM$ is the tangent bundle, and given a coordinate neighbourhood U of M , we choose the frame induced by coordinates $\partial/\partial x^\alpha$, for $\alpha = 1, \dots, \dim(M)$, then the connection matrix is related to the familiar Christoffel symbols:

$$\nabla \frac{\partial}{\partial x^\alpha} = \Gamma_{i\alpha}^\beta dx^i \frac{\partial}{\partial x^\beta}. \quad (\text{B.16})$$

A local section $\sigma = \sigma(x)$ can be written as $\sigma = \xi^\alpha(x) s_\alpha$ for q local functions ξ^1, \dots, ξ^q . Using the properties (B.10, B.11, B.12), we can write the covariant derivative of $\sigma = \xi^\alpha(x) s_\alpha$ as

$$\nabla (\xi^\alpha s_\alpha) = (d\xi^\beta + \xi^\alpha \omega_\alpha^\beta) s_\beta. \quad (\text{B.17})$$

The local section σ is called *horizontal* if $\nabla \sigma = 0$. Horizontal sections defined on open sets U of M do not exist a priori, but horizontal sections along (smooth) *curves* on U always exist, since the condition of being horizontal becomes an ordinary differential equation with smooth right-hand side. By Picard's theorem, there is always a unique and smooth solution for short times, given an initial condition. Given a curve $x(t)$ on U and a corresponding point $(x(0), \xi)$ on $E_{x(0)}$, the unique horizontal local section along $x(t)$ that meets $(x(0), \xi)$ defines a curve $(x(t), \xi(t))$ on E , where $\xi(t) \in E_{x(t)}$. The curve $(x(t), \xi(t))$ obtained by this procedure is called the *horizontal lift* of the curve $x(t)$. Consider the following 1-forms on $E|_U = \pi^{-1}(U)$:

$$\delta \xi^\beta = d\xi^\beta + \xi^\alpha \omega_{i\alpha}^\beta(x) dx^i. \quad (\text{B.18})$$

By construction, if we have a curve on E which is the horizontal lift of a curve on U , then the tangent vectors of the curve on E will be annihilated by the 1-forms $\delta \xi^\beta$. Furthermore, it can be shown that $\delta \xi^\beta$ transforms as a vector under a change of frame: if $s_\alpha(x) \rightarrow s'_\alpha(x) = A_\alpha^\beta(x) s_\beta(x)$, where A_α^β is a $(q \times q)$ invertible matrix of functions on U , then $\delta \xi^\beta = A_\alpha^\beta \delta \xi'^\alpha$.

At each point (x, ξ) of a vector bundle $\pi : E \rightarrow M$, there is a canonically defined *vertical subspace* $VE_{(x, \xi)}$ of the tangent space $T_{(x, \xi)}E$, defined as

$$VE_{(x, \xi)} = \ker(\pi_* : T_{(x, \xi)}E \rightarrow T_x M) = \ker(dx^i). \quad (\text{B.19})$$

Equivalently, $VE_{(x, \xi)}$ is the span of the tangent vectors of curves based at (x, ξ) that do not leave the fibre E_x . Since E_x is a vector space, this gives a canonical isomorphism $VE_{(x, \xi)} \simeq E_x$, which we will suppress in our notation.

We can (noncanonically) define a *horizontal subspace* $HE_{(x, \xi)}$ of $T_{(x, \xi)}E$, such that $VE_{(x, \xi)} \oplus HE_{(x, \xi)} = T_{(x, \xi)}E$, using a connection. It is defined as

$$HE_{(x, \xi)} = \ker(\delta \xi^\beta) = \ker(d\xi^\beta + \xi^\alpha \omega_{i\alpha}^\beta(x) dx^i). \quad (\text{B.20})$$

Equivalently, $HE_{(x, \xi)}$ is the span of tangent vectors of curves based at (x, ξ) , which arose from horizontal lifts of curves on the base manifold M based at x . Since the 1-forms (B.18) transform appropriately under the change of frames, the definition of $HE_{(x, \xi)}$ as the kernel of the 1-forms $\delta \xi^\beta$ is independent of the choice of frame, and only depends on the connection ∇ .

Now we can construct the Riemannian metric on the total space E as follows. Let $X \in T_{(x, \xi)}E$. Since $VE_{(x, \xi)} \oplus HE_{(x, \xi)} = T_{(x, \xi)}E$, there are unique vectors $X_v \in VE_{(x, \xi)}$ and $X_h \in HE_{(x, \xi)}$ such that $X = X_v + X_h$. X_v and X_h are called the *vertical component* and *horizontal component* of X , respectively. Here we use the subscripts v and h to denote the vertical and horizontal components for tangent vectors on E .

In terms of the Riemannian metric g on M and the Riemannian structure h on the vector bundle E , we can define a Riemannian metric G on the total space E as follows:

$$G_{(x, \xi)}(X, Y) = g_x(\pi_* X_h, \pi_* Y_h) + h_x(X_v, Y_v), \quad \text{for } X, Y \in T_{(x, \xi)}E. \quad (\text{B.21})$$

We have suppressed the isomorphism $VE_{(x,\xi)} \simeq E_x$ from the notation. In coordinates, if $h_{\alpha\beta} = h(s_\alpha, s_\beta)$ are the components of the Riemannian structure, then

$$G = g_{ij}dx^i dx^j + h_{\alpha\beta}\delta\xi^\alpha\delta\xi^\beta. \quad (\text{B.22})$$

When $E = TM$ and the connection is the Riemannian connection (also known as the Levi-Civita connection) on M , the metric G is precisely the *Sasaki metric* [34]. We can similarly endow $T^{(N)}M$ with a Riemannian metric, by applying the isomorphism $T^{(N)}M \simeq (T \oplus \cdots \oplus T)M$ using the Riemannian connection on TM (see appendix B.1). Since $(T \oplus \cdots \oplus T)M$ can be endowed with a Riemannian metric (using the direct sum Riemannian structure and the direct sum connection inherited from TM), we can pull this back to a Riemannian metric on $T^{(N)}M$. When $M = \mathbb{R}^n$ with the standard metric δ_{ij} , the metric so constructed on $T^{(N)}M$ coincides with the standard metric on $\mathbb{R}^{n(N+1)}$, since the Christoffel symbols vanish identically.

References

- [1] A. N. Beris and B. J. Edwards. Poisson bracket formulation of viscoelastic flow equations of differential type: A unified approach. *J. Rheol.*, 34:503–538, 1990.
- [2] A. N. Beris and B. J. Edwards. *Thermodynamics of Flowing Systems*. Oxford University Press, Oxford, 1994.
- [3] R. Bird, C. Curtiss, R. Armstrong, and O. Hassager. *Dynamics of Polymeric Liquids, Volume 2: Kinetic Theory*. Wiley, New York, 1987.
- [4] D. W. Condiff and J. S. Dahler. Fluid mechanical aspects of antisymmetric stress. *Phys. Fluids*, 7:842–854, 1964.
- [5] E. Cosserat and F. Cosserat. *Théorie des Corps Déformables*,. A. Hermann et fils, Paris, 1909.
- [6] C. T. J. Dodson and M. S. Radivoiovic. Second-order tangent structures. *Int. J. Theor. Phys.*, 21:151–161, Feb 1982.
- [7] C. T. J. Dodson and M. S. Radivoiovic. Tangent and frame bundles of order two. *An. Stiint. Univ. “Al. I. Cuza” Iasi Sect. I a Mat.(NS)*, 28:63–71, 1982.
- [8] D. G. Ebin and J. Marsden. Groups of diffeomorphisms and the motion of an incompressible fluid. *Ann. Math.*, 92:102–163, 1970.
- [9] B. J. Edwards, A. N. Beris, and M. Grmela. Generalized constitutive equation for polymeric liquid crystals. Part 1. Model formulation using the Hamiltonian (Poisson bracket) formulation. *J. Non-Newton. Fluid Mech.*, 35:51–72, 1990.
- [10] C. P. Enz and L. A. Turski. On the Fokker–Planck description of compressible fluids. *Physica A*, 96:369–378, 1979.
- [11] F. Gay-Balmaz and T. S. Ratiu. The geometric structure of complex fluids. *Adv. Appl. Math.*, 42:176–275, 2009.
- [12] M. Grmela. Hamiltonian dynamics of incompressible elastic fluids. *Phys. Lett. A*, 130:81–86, 1988.
- [13] M. Grmela. Hamiltonian dynamics of elastic fluids: Ericksen stresses. *Phys. Lett. A*, 137:342–348, 1989.
- [14] D. D. Holm. Euler–Poincaré dynamics of perfect complex fluids. In J. Marsden, P. Newton, P. Holmes, and A. Weinstein, editors, *Geometry, Mechanics, and Dynamics: Volume in Honor of the 60th Birthday of J.E. Marsden*, pages 114–168, New York, 2002. Springer.
- [15] D. D. Holm, J. E. Marsden, and T. S. Ratiu. The Euler–Poincaré equations and semidirect products with applications to continuum theories. *Adv. Math.*, 137:1–81, 1998.
- [16] J. Jost. *Riemannian Geometry and Geometric Analysis*. Springer, Berlin; Heidelberg, 2006.
- [17] B. Khesin and R. Wendt. *The Geometry of Infinite-Dimensional Groups*. Springer, Berlin; Heidelberg, 2008.
- [18] S. Kim and S. J. Karrila. *Microhydrodynamics*. Dover, New York, 2005.

- [19] A. T. Mackay and T. N. Phillips. On the derivation of macroscopic models for compressible viscoelastic fluids using the generalized bracket framework. *J. Non-Newton. Fluid Mech.*, 266:59–71, 2019.
- [20] J. E. Marsden, T. Ratiu, and A. Weinstein. Semidirect products and reduction in mechanics. *T. Am. Math. Soc.*, 281:147–177, 1984.
- [21] J. E. Marsden, T. Ratiu, and A. J. Weinstein. Reduction and Hamiltonian structures on duals of semidirect product Lie algebras. *Contemp. Math.*, 28:55–100, 01 1984.
- [22] J. E. Marsden and T. S. Ratiu. *Introduction to Mechanics and Symmetry*. Springer, New York, 2013.
- [23] J. E. Marsden, A. Weinstein, T. Ratiu, R. Schmid, and R. G. Spencer. Hamiltonian systems with symmetry, coadjoint orbits and plasma physics. In *Proceedings of the IUTAM-ISIMM symposium on modern developments in analytical mechanics, Vol. I (Torino, 1982)*, pages 289–340, 1983.
- [24] P. J. Morrison. Some observations regarding brackets and dissipation. Center for Pure and Applied Mathematics Report PAM-228, University of California, Berkeley, 1984.
- [25] P. J. Morrison. A paradigm for joined Hamiltonian and dissipative systems. *Physica D*, 18:410–419, 1986.
- [26] P. J. Morrison. Hamiltonian description of the ideal fluid. *Rev. Mod. Phys.*, 70:467–521, 1998.
- [27] P. J. Morrison and J. M. Greene. Noncanonical Hamiltonian density formulation of hydrodynamics and ideal magnetohydrodynamics. *Phys. Rev. Lett.*, 45:790–794, Sep 1980.
- [28] M. Renardy. *Mathematical Analysis of Viscoelastic Flows*. Society for Industrial and Applied Mathematics, Philadelphia, 2000.
- [29] R. E. Rosensweig. *Ferrohydrodynamics*. Cambridge University Press, Cambridge, 1985.
- [30] R. Salmon. Hamiltonian fluid mechanics. *Annu. Rev. Fluid Mech.*, 20:225–256, 1988.
- [31] M. I. Shliomis. Magnetic fluids. *Soviet Phys. Uspekhi*, 17:153–169, 1974.
- [32] L. W. Tu. *Differential Geometry*. Springer International Publishing, Cham, Switzerland, 2017.
- [33] A. Weinstein. The local structure of Poisson manifolds. *J. Differ. Geom.*, 18:523–557, 1983.
- [34] K. Yano and S. Ishihara. *Tangent and Cotangent Bundles: Differential Geometry*. Dekker, New York, 1973.
- [35] V. E. Zakharov and E. A. Kuznetsov. Hamiltonian formalism for nonlinear waves. *Physics–Uspekhi*, 40:1087–1116, 1997.