Geometrical Methods in Dynamics of Complex Fluids and Kinetic Theory



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Abstract

In this thesis, we study three applications of the noncanonical Hamiltonian formalism to fluid dynamics and the kinetic theory of gases and polymers.

The first application is in polymer kinetic theory. A common model for a polymer solution is a suspension of multibead-chains in a Newtonian fluid. The configuration of the chains is described by a kinetic distribution function. We consider a double bracket formulation for the dynamics of this suspension. The reversible part is governed by a semidirect Lie–Poisson bracket, and the irreversible part is governed by a symmetric dissipation bracket. The Poisson bracket captures the kinematics of the beads being advected as Lagrangian markers. We find that chains with three or more beads can transmit angular momentum by bending, which produces an asymmetric couple stress. These terms support couple stress boundary layers at rigid boundaries. Finally, we derive closed macroscopic models that describe suspensions of Hookean multibead-chains.

The second application is in gas kinetic theory. An ideal gas is described by the Boltzmann equation, which becomes a noncanonical Hamiltonian system if we neglect collisions. A long-standing problem in gas kinetic theory is the derivation of reduced hydrodynamic descriptions. We analyse some of these reductions using Poisson geometry. In particular, we give a manifestly Hamiltonian derivation of the compressible Euler equations from kinetic theory using a Poisson map and an approximation to the Hamiltonian. We extend these results to electrostatic plasmas described by the Vlasov–Poisson system.

The final application is to active matter. We consider the ideal dynamics of a suspension of active rod-like swimmers. We establish a novel analogy between the active suspension and magnetohydrodynamics (MHD) in a nonlinear media. The magnetic field becomes the orientation field for the swimmers. Its magnitude then becomes a gauge degree of freedom, which we describe using Poisson geometry. The active suspension shares the noncanonical Hamiltonian formulation with MHD. Using the energy-Casimir and energy-momentum methods, we find force-free fields and finite amplitude Alfvén waves in the active suspension.

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Chapter 1

Introduction

1.1 From microscopic to macroscopic physics

The formulation and analysis of models at different levels of description for a physical system is a classical topic in continuum physics. There are two main classes of models. The first are *macroscopic* models that describe the system using fields over the spatial location $\mathbf{x}$ only. The second are *microscopic* models that consider additional internal degrees of freedom in the system. One often derives macroscopic models by making suitable approximations in an underlying microscopic model, for example by imposing constraints or considering asymptotic limits of some small parameters.

A well-known example is the dynamics of a monatomic ideal gas. The *Navier–Stokes–Fourier* equations constitute a macroscopic hydrodynamic model formulated in terms of mass, momentum and energy conservation. A typical set of variables consists of the *mass density* $\rho(\mathbf{x}, t)$, the *fluid velocity* $\mathbf{u}(\mathbf{x}, t)$ and the *temperature*[1] $\theta(\mathbf{x}, t)$ of the gas. They evolve in time as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{1.1.1a}$$

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla (\rho\theta) + \nabla \cdot \boldsymbol{\pi}, \tag{1.1.1b}$$

$$\frac{3}{2}\rho \left(\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta \right) + \rho\theta \nabla \cdot \mathbf{u} = \boldsymbol{\pi} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q}, \tag{1.1.1c}$$

where $\boldsymbol{\pi}$ is the *viscous stress* and $\mathbf{q}$ is the *diffusive heat flux*. The viscous stress and diffusive heat flux are unknown from first principles, and one must assume constitutive relations to close the system (1.1.1a-c). For the Navier–Stokes–Fourier equations, these constitutive

[1] The temperature θ is given in so-called energy units, where the Boltzmann constant k_B has been absorbed in its definition. The gas pressure in these units is $\rho\theta$.

relations are

$$\pi = \mu\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right) + \left(\zeta - \frac{2}{3}\mu\right)(\nabla\cdot\mathbf{u})\mathbf{I}, \quad \mathbf{q} = -\kappa\nabla\theta, \tag{1.1.2}$$

where μ is the shear viscosity, ζ is the bulk viscosity and κ is the thermal diffusivity of the gas. The coefficients μ, ζ, κ, which can be functions of ρ and θ, are determined by the internal properties of the gas. In the time-reversible limit where the viscous and diffusive effects can be ignored ($\mu = \zeta = \kappa = 0$), the equations (1.1.1a-c) becomes the *compressible Euler equations*.

The *entropy density*[2] $s = -\rho\log(\rho\theta^{-3/2})$ of the gas evolves in time as

$$\frac{\partial s}{\partial t} + \nabla\cdot(s\mathbf{u}) = \frac{1}{\theta}\left(\boldsymbol{\pi} : \nabla\mathbf{u} - \nabla\cdot\mathbf{q}\right). \tag{1.1.3}$$

The variables $\rho, \mathbf{u}, s$ also form a closed set of evolution equations. The entropy density s is often preferred over the temperature θ when we consider the compressible Euler equations, because s (1.1.3) evolves just like the density ρ in the absence of viscous and diffusive effects.

On the other hand, *kinetic theory* provides an alternative microscopic description of the monatomic ideal gas. In kinetic theory, we consider the precise distribution of velocities of the gas particles instead of just their macroscopic thermodynamic and statistical properties. The 1-*particle distribution function* $f(\mathbf{x}, \mathbf{v}, t)$, which describes the phase-space density of gas particles at position $\mathbf{x}$ with velocity $\mathbf{v}$, evolves in time according to the *Boltzmann equation* [31, 32, 33, 35, 77, 89, 150]

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{x}} = C[f, f]. \tag{1.1.4}$$

The term $C[f, f]$ is a symmetric bilinear operator known as the *collision operator*. The macroscopic variables $\rho, \mathbf{u}, \theta$ introduced earlier are related to the distribution function by

$$\rho = \int d^3v\ f, \tag{1.1.5a}$$

$$\rho\mathbf{u} = \int d^3v\ \mathbf{v}f, \tag{1.1.5b}$$

$$\rho\left(\frac{1}{2}|\mathbf{u}|^2 + \frac{3}{2}\theta\right) = \int d^3v\ \frac{1}{2}|\mathbf{v}|^2 f, \tag{1.1.5c}$$

assuming for simplicity that the gas particles have unit mass. In general, velocity-space integrals of the distribution function f are known as *moments* of f. The moments in

[2] We use the physicists' sign convention for the entropy density in the introduction, so that the entropy is a non-decreasing function in time. The opposite sign convention is used in chapter **4**.

(1.1.5a-c) are special because the collision operator $C[f,f]$ in (1.1.4) satisfies

$$\int d^3v \begin{pmatrix} 1 \\ \mathbf{v} \\ |\mathbf{v}|^2 \end{pmatrix} C[f,f] = 0, \tag{1.1.6}$$

so these moments are conserved under collisions. We can thus derive equations (1.1.1a-c) by taking the moments $(1, \mathbf{v}, |\mathbf{v}|^2)$ of the Boltzmann equation (1.1.4). Additionally, the collision operator satisfies

$$C[f_m, f_m] = 0 \text{ for all } f_m(\mathbf{x},\mathbf{v},t) = \rho(\mathbf{x},t)\exp\left(-\frac{|\mathbf{v}-\mathbf{u}(\mathbf{x},t)|^2}{2\theta(\mathbf{x},t)}\right). \tag{1.1.7}$$

Distribution functions of the form f_m in (1.1.7) are known as *Maxwellian* distribution functions. Each distribution function f has an associated local Maxwellian f_m that has the same $(1, \mathbf{v}, |\mathbf{v}|^2)$-moments (1.1.5a-c) as f. This invites a decomposition of f into a local Maxwellian f_m and a non-Maxwellian part h:

$$f = f_m + h, \quad \text{where } \int d^3v \begin{pmatrix} 1 \\ \mathbf{v} \\ |\mathbf{v}|^2 \end{pmatrix} h = 0. \tag{1.1.8}$$

The viscous stress $\boldsymbol{\pi}$ and the heat flux $\mathbf{q}$ now depend solely on the currently unknown non-Maxwellian part h:

$$\boldsymbol{\pi} = -\int d^3v\, (\mathbf{v}-\mathbf{u})(\mathbf{v}-\mathbf{u})h, \quad \mathbf{q} = \int d^3v\, \frac{1}{2}|\mathbf{v}-\mathbf{u}|^2(\mathbf{v}-\mathbf{u})h, \tag{1.1.9}$$

so the system of equations (1.1.1a-c) for $\rho, \mathbf{u}, \theta$ (1.1.5a-c) is not closed.

We can obtain a closed set of equations for the hydrodynamic variables $\rho, \mathbf{u}, \theta$ by taking the strongly collisional limit. There are two timescales in the Boltzmann equation (1.1.4). The first is the macroscopic timescale T for hydrodynamic processes. The second is the mean free time between collisions τ. These timescales are related to the terms in the Boltzmann equation (1.1.4) as

$$\frac{1}{T} \sim \frac{1}{f}\frac{\partial f}{\partial t}, \frac{1}{f}\mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{x}}, \quad \frac{1}{\tau} \sim \frac{1}{f}C[f,f], \tag{1.1.10}$$

and the *Knudsen number* is defined as the ratio $\mathrm{Kn} = \tau/T$. In the strongly collisional limit $\mathrm{Kn} \to 0$, the mean free time is vanishingly small compared to the macroscopic time. The collisional term on the right-hand side of (1.1.4) then becomes formally large, so one expects $f \simeq f_m$ due to property (1.1.7). Due to property (1.1.6), the moments in (1.1.5a-c) should evolve on the macroscopic timescale T, while any other moment should evolve on

the mean free time τ. This is formalised in the multiple-scales expansion known as the *Chapman–Enskog expansion* [33, 35, 89]:

$$t = t_0 + \mathrm{Kn}^{-1}\, t_1 + \ldots, \quad \text{so that } \frac{\partial}{\partial t} = \frac{\partial}{\partial t_0} + \mathrm{Kn}\, \frac{\partial}{\partial t_1} + \ldots, \tag{1.1.11a}$$

$$h = \mathrm{Kn}\, h^{(1)} + \mathrm{Kn}^2\, h^{(2)} + \ldots, \quad \int d^3v \begin{pmatrix} 1 \\ \mathbf{v} \\ |\mathbf{v}|^2 \end{pmatrix} h^{(k)} = 0 \text{ for } k = 1, 2, \ldots, \tag{1.1.11b}$$

where all functions of t are now treated as functions of a set of independent time variables $t_0, t_1, \ldots$. Let us expand the Boltzmann equation (1.1.4) order by order:

$$O(\mathrm{Kn}^{-1}): \qquad 0 = C[f_m, f_m], \tag{1.1.12a}$$

$$O(1): \qquad \frac{\partial f_m}{\partial t_0} + \mathbf{v} \cdot \frac{\partial f_m}{\partial \mathbf{x}} = 2C[f_m, h^{(1)}], \tag{1.1.12b}$$

$$O(\mathrm{Kn}): \qquad \frac{\partial f_m}{\partial t_1} + \frac{\partial h^{(1)}}{\partial t_0} + \mathbf{v} \cdot \frac{\partial h^{(1)}}{\partial \mathbf{x}} = 2C[f_m, h^{(2)}] + C[h^{(1)}, h^{(1)}], \tag{1.1.12c}$$

and so on. The term $2C[f_m, h^{(1)}]$ on the right-hand side of (1.1.12b) is known as the *linearised collision operator*. The leading order equation (1.1.12a) gives $f = f_m$, or equivalently $h = 0$. Taking the moments $(1, \mathbf{v}, |\mathbf{v}|^2)$ of (1.1.12b) then gives the compressible Euler equations i.e. the system (1.1.1a-c) with $\boldsymbol{\pi} = \mathbf{q} = 0$. To obtain $O(\mathrm{Kn})$ corrections to the compressible Euler equations, we need to solve for $h^{(1)}$ using (1.1.12b). The left-hand side of (1.1.12b) can be written in terms of $\rho, \mathbf{u}, \theta$ and their spatial derivatives, because $\partial_{t_0}(\rho, \mathbf{u}, \theta)$ and hence $\partial_{t_0} f_m$ are given by the compressible Euler equations. We can then solve for $h^{(1)} = h^{(1)}(\rho, \mathbf{u}, \theta, \nabla\mathbf{u}, \nabla\theta)$ by inverting the linear operator $2C[f_m, h]$ on the right-hand side of (1.1.12b) using the solvability conditions (1.1.11b). The $O(\mathrm{Kn})$ corrections $\mathrm{Kn}\, \partial_{t_1}(\rho, \mathbf{u}, \theta)$ are then found from taking the moments $(1, \mathbf{v}, |\mathbf{v}|^2)$ of (1.1.12c).

The explicit form of $h^{(1)}$ depends on the collision operator. For example, it is common to replace the linearised collision operator $2C[f_m, h^{(1)}]$ in (1.1.12b) with the Bhatnagar–Gross–Krook (BGK) collision operator[3] [18]

$$2C[f_m, h] \text{ is replaced by } -\frac{1}{\tau}(f - f_m) = -\frac{1}{\tau} h, \tag{1.1.13}$$

where τ is the mean free time. Solving for $h^{(1)}$ then returns the expressions (1.1.2) for $\boldsymbol{\pi}$ and $\mathbf{q}$, with the coefficients μ, ζ, κ given by

$$\mu = \tau\rho\theta, \quad \zeta = 0, \quad \kappa = \frac{5}{2}\tau\rho\theta. \tag{1.1.14}$$

[3]The BGK collision operator is not linear in f because the dependence of f_m on f is highly nonlinear, but it is always linear in h.

Another example is when $C[f, f]$ is the collision operator for Maxwell molecules, where particle collisions are modelled by an inverse fifth-power repulsive force. By inverting the corresponding linearised collision operator $2C[f_m, h]$, one recovers the constitutive relations (1.1.2, 1.1.14), with a slightly different numerical coefficient for κ [77, 89]. The Boltzmann equation (1.1.4) thus provides a microscopic model from which the Navier–Stokes–Fourier equations (1.1.1a-c) can be derived in the strongly collisional limit $\mathrm{Kn} \to 0$.

The derivation of macroscopic models from microscopic models is also a recurring theme in the theory of polymer suspensions [21, 51, 148]. An elementary model of a polymer molecule is a pair of beads connected by a massless elastic spring. In the kinetic theory of such a polymer suspension, one considers the distribution function $\psi(\mathbf{x}, \mathbf{y}, t)$, the expected number density of polymer molecules at spatial location $\mathbf{x}$ with end-to-end extension $\mathbf{y}$. Unlike the kinetic theory of gases, the fluid velocity $\mathbf{u}(\mathbf{x}, t)$ is not directly related to ψ; instead, we have a coupled system of evolution equations for both variables $\mathbf{u}$ and ψ. The problem of deriving macroscopic models then involves eliminating the $\mathbf{y}$-dependence in the system, either exactly or under some approximation scheme. This is usually achieved by finding a finite subset of $\mathbf{y}$-integrals of ψ, which we also call *moments*, that produces a closed set of evolution equations. For example, in a popular model where the springs are Hookean, the moment $\int d^3y\, \mathbf{y}\mathbf{y}\psi$ provides a closed system. We will revisit this scenario again in section **1.3** and later in chapter **3**.

In this thesis, we consider the *noncanonical Hamiltonian formulation* of these continuum systems. In the limit of vanishing time-irreversible effects such as diffusion and dissipation, many continuum systems can be formulated as Hamiltonian systems on infinite-dimensional spaces of field variables [94, 137, 153]. Examples include ordinary fluid dynamics [127, 128, 138, 153, 154], magnetohydrodynamics (MHD) [6, 94, 127, 128, 129, 138], dynamics of complex fluids [16, 17, 57, 69, 78, 79, 119] and kinetic theory of plasmas [72, 94, 126, 130]. The noncanonical Hamiltonian formulation is a powerful tool that elucidates mathematical properties and provide physical insight. In this chapter, we discuss four main benefits of such a formulation:

1. The noncanonical Hamiltonian formulation is useful for constructing models for complex fluids with desirable properties. For example, the *semidirect product Lie–Poisson formulation* captures complex fluids where the internal structure is materially advected by the fluid (section **1.3**).

2. The noncanonical Hamiltonian formulation reveals genuinely nonlinear properties of the system, such as symmetries and exact conservation laws. Moreover, the *energy-Casimir* and the *energy-momentum* methods provide a systematic way to find exact

steady-state and nonlinear travelling wave solutions from a noncanonical Hamiltonian formulation, and sometimes prove their nonlinear stability (section **1.4**).

3. Reduced Hamiltonian systems can be derived from a more primitive Hamiltonian system using tools from *Poisson geometry*, so as to retain important structural properties (section **1.5**). Such derivations can either be exact or involve approximations, and the geometric perspective elucidates how the approximations can be made in a manifestly Hamiltonian way.

4. We can also treat systems with both reversible and dissipative parts using the *double bracket formulation*, where an additional symmetric bracket is introduced alongside the Poisson bracket used in noncanonical Hamiltonian mechanics. The double bracket formulation is compatible with principles in non-equilibrium thermodynamics (section **1.3**), and the nonlinear stability results from the energy-Casimir method carry over under appropriate conditions (section **1.4**).

The noncanonical Hamiltonian formulation thus extends our ability to analysis continuum systems beyond the traditional tools of linearisation and perturbation expansions, while also offering nuanced insight to common approximations and constitutive laws in continuum mechanics.

1.2 Canonical and noncanonical Hamiltonian mechanics

We give a brief introduction to noncanonical Hamiltonian mechanics in this section. We will revisit noncanonical Hamiltonian mechanics in much more detail in chapter **2**.

In the Hamiltonian formulation of classical mechanics (see e.g. [10]), a state $(\mathbf{q}, \mathbf{p}) \in \mathbb{R}^{2n}$ in phase space evolves according to Hamilton's equations of motion

$$\frac{d\mathbf{q}}{dt} = \frac{\partial H}{\partial \mathbf{p}}, \tag{1.2.1a}$$

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{q}}, \tag{1.2.1b}$$

where $H = H(\mathbf{q}, \mathbf{p})$ is the *Hamiltonian* function, which is usually the total energy of the system. Any phase-space function $F = F(\mathbf{q}, \mathbf{p})$ evolves in time as

$$\frac{dF}{dt} = \{F, H\}, \tag{1.2.2}$$

where $\{\cdot, \cdot\}$ is the *canonical Poisson bracket*:

$$\{F, H\} = \frac{\partial F}{\partial \mathbf{q}} \cdot \frac{\partial H}{\partial \mathbf{p}} - \frac{\partial H}{\partial \mathbf{q}} \cdot \frac{\partial F}{\partial \mathbf{p}}. \tag{1.2.3}$$

The equivalence between the Poisson bracket formulation (1.2.2) and Hamilton's equations (1.2.1a,b) comes from considering arbitrary F and using the chain rule.

Noncanonical Hamiltonian mechanics is an abstract generalisation of the system (1.2.2), where instead of using the classical phase space $\mathbb{R}^{2n}$ and the canonical Poisson bracket (1.2.3), one uses an abstract configuration space M with an abstract Poisson bracket [94, 137, 153]. Usually, M is a smooth manifold, and the Poisson bracket is a bilinear skew-symmetric operator on smooth functions $f, g \mapsto \{f, g\}$ satisfying the Leibniz and Jacobi identities

$$\{f, gh\} = \{f, g\}h + g\{f, h\}, \tag{1.2.4a}$$

$$\{\{f, g\}, h\} + \{\{g, h\}, f\} + \{\{h, f\}, g\} = 0, \tag{1.2.4b}$$

for all smooth functions f, g, h on M. A configuration space M that is equipped with a Poisson bracket is known as a *Poisson manifold* [28, 107, 114, 183]. The adjective "noncanonical" refers to the fact that canonical coordinates $(\mathbf{q}, \mathbf{p})$ do not necessarily exist on Poisson manifolds, even locally. An elementary example of a noncanonical Hamiltonian system is the dynamics of a free rigid body. The angular momentum $\mathbf{L} \in \mathbb{R}^3$ of a rigid body, measured in the frame of the body, obeys Euler's rotation equation

$$\frac{d\mathbf{L}}{dt} = -(I^{-1}\mathbf{L}) \times \mathbf{L}, \tag{1.2.5}$$

where I is the inertia tensor of the rigid body in the body frame (which is constant in time), and $\times$ is the cross product on $\mathbb{R}^3$. The system (1.2.5) can be written as a noncanonical Hamiltonian system:

$$\frac{d\mathbf{L}}{dt} = \{\mathbf{L}, H\}_\times, \tag{1.2.6}$$

where $H(\mathbf{L}) = \mathbf{L}I^{-1}\mathbf{L}/2$ is the total energy of the system, and

$$\{F, H\}_\times := -\mathbf{L} \cdot \left(\frac{\partial F}{\partial \mathbf{L}} \times \frac{\partial H}{\partial \mathbf{L}}\right) \tag{1.2.7}$$

is a noncanonical Poisson bracket on $\mathbb{R}^3$. For any $F = F(\mathbf{L})$, we have

$$\left\{F, |\mathbf{L}|^2\right\}_\times = -2\mathbf{L} \cdot \left(\frac{\partial F}{\partial \mathbf{L}} \times \mathbf{L}\right) = 0, \tag{1.2.8}$$

so there can be non-constant functions such as $C = |\mathbf{L}|^2$ whose Poisson bracket with any other function vanishes, unlike the canonical Hamiltonian formulation. Such C are called *Casimir functions*, and they play an important role in noncanonical Hamiltonian mechanics. For instance, Casimir functions are automatically constants of motion. For the free rigid body

(1.2.5), this immediately implies that the trajectory of $\mathbf{L}(t)$ is confined to the intersection of the inertial ellipsoid $\mathbf{L}(t)I^{-1}\mathbf{L}(t)/2 = H(t=0)$ and the sphere $|\mathbf{L}(t)|^2 = |\mathbf{L}(t=0)|^2$.

The connection between canonical and noncanonical Hamiltonian mechanics is provided by the *Weinstein splitting theorem* [183]. The general case is considered in section **2.1.1**. Here we illustrate a special case by changing from cartesian coordinates to the curvilinear coordinates $(|\mathbf{L}|, \varphi, L_z)$ defined by

$$\mathbf{L} = \left(\sqrt{|\mathbf{L}|^2 - L_z^2}\cos\varphi, \sqrt{|\mathbf{L}|^2 - L_z^2}\sin\varphi, L_z\right), \tag{1.2.9}$$

which transforms the cross-product (1.2.7) to "canonical form"

$$\{F, H\}_\times = \frac{\partial F}{\partial \varphi}\frac{\partial H}{\partial L_z} - \frac{\partial H}{\partial \varphi}\frac{\partial F}{\partial L_z}. \tag{1.2.10}$$

We can imagine $\mathbb{R}^3$ to be a union of spheres, each of which equipped with a pair of canonically conjugate coordinates φ, L_z, so that the Hamiltonian $H = H(|\mathbf{L}|, \varphi, L_z)$ generates one set of Hamilton's equations (1.2.1a,b) for each value of $|\mathbf{L}| > 0$. The only place where this picture breaks down is $\mathbf{L} = 0$, because $\{F, H\}_\times(\mathbf{L} = 0)$ vanishes identically. The spheres in this example are known as *symplectic leaves*, and they are labelled by the values of the Casimir function $|\mathbf{L}|^2$. Intuitively, we can think of the configuration space of a noncanonical Hamiltonian system as a union of canonical phase spaces, each of appropriate dimension, with the degenerate or "noncanonical" directions labelled by the Casimir functions. Strictly speaking, this intuition is incorrect – we have just seen it fail at the point $\mathbf{L} = 0$ in the previous example – but it gives an instructive heuristic picture.

1.3 Noncanonical Hamiltonian mechanics in model formulation

Noncanonical Hamiltonian mechanics is a very powerful tool in model formulation for complex fluids. A *complex fluid* is a fluid with internal structure. Common examples of complex fluids are polymer solutions [20, 21, 51, 148], flowing liquid crystals [60, 61, 116, 117, 166], ferrofluids [149, 158, 161], and solutions of swimming bacteria [52, 53, 75, 90, 147, 162, 175]. The internal structure of the fluid is perturbed by the fluid flow, which in turn exerts an additional stress back on the fluid. A typical set of governing equations for an incompressible complex fluid[4] is

$$\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla P + \nu\nabla^2\mathbf{u} + \nabla\cdot\boldsymbol{\sigma}[\mathbf{u}, \boldsymbol{\psi}], \qquad \nabla\cdot\mathbf{u} = 0, \tag{1.3.1}$$

$$\partial_t \boldsymbol{\psi} = L[\mathbf{u}, \boldsymbol{\psi}] + R[\boldsymbol{\psi}], \tag{1.3.2}$$

[4]One proceeds entirely analogously for a compressible fluid by lifting the restriction $\nabla\cdot\mathbf{u} = 0$ and introducing the appropriate equation for the fluid mass density ρ.

where $\mathbf{u}$ is the fluid velocity field, P is the pressure, ν is the (Newtonian) kinematic viscosity, and $\boldsymbol{\psi}$ is some set of variables describing the internal structure of the complex fluid. The term $L[\mathbf{u}, \boldsymbol{\psi}]$ in (1.3.2) describes the advection of the internal structure by the fluid flow, and the term $R[\boldsymbol{\psi}]$ describes internal effects of the internal structure, such as Brownian diffusion for suspended rigid bodies, or relaxation effects in a flowing liquid crystal.

There are two main classes of models for such a complex fluid. The first is an *internal state variable* model, in which $\boldsymbol{\psi} = \boldsymbol{\psi}(\mathbf{x}, t)$ are macroscopic field variables over the spatial domain only. The second class is a *kinetic model*, where $\boldsymbol{\psi}$ are functions of both the spatial location $\mathbf{x}$ and some variable y describing the precise internal configuration. For example, if the complex fluid is a suspension of rigid bodies, then $y \in SO(3)$ would describe the orientation of the rigid body at $\mathbf{x}$ relative to a reference orientation. In both cases, the internal structure in turn exerts an additional *non-Newtonian stress* $\boldsymbol{\sigma}[\mathbf{u}, \boldsymbol{\psi}]$ on the fluid.

We break down the modelling of a complex fluid into the following steps:

1. Postulate a set of variables $\boldsymbol{\psi}$, macroscopic or microscopic, that describes the internal structure of the fluid.

2. Postulate the form of the fluid advection effects $L[\mathbf{u}, \boldsymbol{\psi}]$ and internal effects $R[\boldsymbol{\psi}]$ in the evolution equation (1.3.2) for $\boldsymbol{\psi}$.

3. Postulate the form of the non-Newtonian stress $\boldsymbol{\sigma}[\mathbf{u}, \boldsymbol{\psi}]$ that the internal structure exerts on the fluid.

In the traditional phenomenological approach (see e.g. [20]), one takes the non-Newtonian stress as the internal state variable ($\boldsymbol{\sigma} = \boldsymbol{\psi}$) and postulates a time evolution equation for $\boldsymbol{\sigma}$, which is a special case of the framework above.

Let us temporarily ignore the Newtonian viscosity ν and the internal relaxation terms $R[\boldsymbol{\psi}]$ in our complex fluid model (1.3.1, 1.3.2). In the absence of these time-irreversible effects, we expect the system to conserve the total energy

$$H[\mathbf{u}, \boldsymbol{\psi}] = \int d^3x \, \left(\frac{1}{2}|\mathbf{u}|^2 + U[\boldsymbol{\psi}] \right), \tag{1.3.3}$$

where $U[\boldsymbol{\psi}]$ is the internal energy density pertaining to the internal structure of the fluid. As a result of this conservation law, the non-Newtonian stress $\boldsymbol{\sigma}$ and the advection term $L[\mathbf{u}, \boldsymbol{\psi}]$ cannot be independently postulated. The physical principal behind this is Newton's third law – under an arbitrary fluid displacement, the work done by the fluid on the internal structure, calculated from $L[\mathbf{u}, \boldsymbol{\psi}]$, must balance the work done by the internal structure on the fluid, calculated from the non-Newtonian stress $\boldsymbol{\sigma}$.

In the dynamics of complex fluids, we often encounter systems where the internal structure is advected by the fluid flow as a set of *Lagrangian markers*. The concept of Lagrangian markers is best explained by the label-to-particle map construction in fluid dynamics [13, 112, 153, 154]. Consider a *label space* $M_0 \simeq \mathbb{R}^3$, consisting of labels $\mathbf{a} \in M_0$ attached to the domain at $t = 0$. We denote our physical space by $M \simeq \mathbb{R}^3$, with $\mathbf{x} \in M$. The flow of the fluid is described by a time-dependent diffeomorphism $\boldsymbol{\chi}_t : M_0 \to M$, with the Eulerian velocity given as $\mathbf{u}(\mathbf{x}, t) = \partial_t \boldsymbol{\chi}_t \circ \boldsymbol{\chi}_t^{-1}$. This construction is also widely used in solid mechanics [122], where M_0 is called the reference configuration, and the map $\boldsymbol{\chi_t} : M_0 \to M$ is called the deformation mapping.

A Lagrangian marker is a point on the label space M_0 that evolves in time along the flow $\boldsymbol{\chi}_t$. Materially advected objects in the fluid can often be thought of as composite objects made of Lagrangian markers. For example, a pair of Lagrangian markers connected by a small elastic spring, which is a common model for a suspended polymer in a fluid, can be thought of as an infinitesimal line segment or tangent vector on M_0. Let us denote its centre of mass by $\mathbf{a}$ and its end-to-end displacement vector by $\mathbf{b}$ in label space. Its centre of mass $\mathbf{x}(t)$ and end-to-end displacement $\mathbf{y}(t)$ in physical space at time t would then be

$$\mathbf{x}(t) = \boldsymbol{\chi}_t(\mathbf{a}), \quad \mathbf{y}(t) = D\boldsymbol{\chi}_t|_{\mathbf{a}}\mathbf{b}, \tag{1.3.4}$$

where $D\boldsymbol{\chi}_t|_{\mathbf{a}}$ is the Jacobian matrix of $\boldsymbol{\chi}_t$ evaluated at $\mathbf{a}$. By postulating that the internal structure is advected as a composite Lagrangian marker of appropriate type, we have fixed the term $L[\mathbf{u}, \boldsymbol{\psi}]$ in (1.3.2). Given that the energy H (1.3.3) is conserved in the absence of dissipation, we should then be able to derive the form of $\boldsymbol{\sigma}$ from Newton's third law, which completes the formulation of our complex fluid model.

The situation described above is conveniently captured by the *semidirect product Lie–Poisson formulation*, which was extensively studied by Marsden et al. [127, 128]. In this formulation, one considers a noncanonical Hamiltonian system on the dual space $(\mathrm{Vect}(M) \ltimes L)^*$ of the semidirect product Lie algebra $\mathrm{Vect}(M) \ltimes L$, where $\mathrm{Vect}(M)$ is the Lie algebra of vector fields on M, and L is an appropriate space of composite Lagrangian markers on which $\mathrm{Vect}(M)$ acts. The Poisson bracket on this space guarantees that $\boldsymbol{\psi}$ evolves according to being advected as a field of composite Lagrangian markers under any Hamiltonian H (1.3.3), and provides a straightforward way to compute the stress $\boldsymbol{\sigma}$ from the postulated total energy [17, 79].

The Poisson bracket formulation is a convenient tool that models the conservative, or reversible, part of the dynamics. A common extension that captures dissipative effects is the *double bracket formulation* [16, 17, 57, 78, 79, 119, 135, 136], where one introduces a

symmetric positive semidefinite bracket $(\cdot,\cdot)$ so that the time evolution (1.2.2) is replaced by

$$\frac{dF}{dt} = \{F, A\} - (F, A), \tag{1.3.5}$$

and the Hamiltonian H is now replaced by the *available energy* A. The double bracket system (1.3.5) constitutes a model for non-equilibrium thermodynamics. We discuss this in connection with other properties of noncanonical Hamiltonian systems in section **2.4**. For example, the non-equilibrium thermodynamics of a closed system can be modelled by taking $A = H - S$, where S is a Casimir functional that quantifies the entropy of the system. By choosing a symmetric bracket that satisfies $(F, H) = 0$ for all functionals F, we obtain a system where

$$\frac{dH}{dt} = 0, \quad \frac{dS}{dt} \geq 0, \quad \frac{dA}{dt} \leq 0, \tag{1.3.6}$$

so that energy is conserved, entropy is non-decreasing, and available energy is non-increasing. A model for a complex fluid that is constructed in an appropriate double bracket formulation (1.3.5) will automatically obey such thermodynamic principles.

In chapter **3**, we present the author's work [41], where the double bracket formulation is used to construct new models for multibead-chain suspensions. The reversible part of the models come from a semidirect product Lie–Poisson formulation, so the non-Newtonian stress on the fluid is directly obtained from the internal energy of the chains. These multibead-chains are composite Lagrangian markers that can *bend*, and hence are sensitive to higher spatial derivatives of the fluid velocity $\mathbf{u}$, which in particular includes the vorticity gradient. As a result, there is net transmission of angular momentum across the chains, and the stress on the fluid is *asymmetric*, leading to a microscopic realisation of a *generalised Cosserat continuum* [43, 45, 58, 149, 198]. The work [41] is an example of how new physical effects can be modelled using the semidirect product Lie–Poisson and double bracket formulations.

1.4 Solutions of a noncanonical Hamiltonian system

Finding a noncanonical Hamiltonian formulation for a system opens up the possibility for a systematic investigation of its steady-state and nonlinear wave solutions. These solutions are obtained respectively from the *energy-Casimir* and *energy-momentum* methods, which are readily available tools in noncanonical Hamiltonian mechanics that formulate the problem of finding such solutions in terms of variational principles. These methods are considered in detail in section **2.4** – here we give a brief overview with intuitive explanations showing their power.

The *energy-Casimir method* obtains steady-state solutions of the noncanonical Hamiltonian system as the critical points of an appropriate variational principle, which has found many applications in geophysical fluid dynamics and plasma physics [91, 94, 137, 154, 160]. For simplicity, let us take a finite-dimensional configuration space $M = \mathbb{R}^n$ with coordinates $z^1, \ldots, z^n$ and Poisson bracket (using the summation convention)

$$\{F, H\} = \Pi^{ij}(z)\frac{\partial F}{\partial z^i}\frac{\partial H}{\partial z^j}, \tag{1.4.1}$$

where $\Pi^{ij}(z)$ is an antisymmetric matrix of functions known as the Poisson tensor[5]. The dynamics generated by the Hamiltonian function $H(z)$ is then

$$\frac{dz^i}{dt} = \Pi^{ij}\frac{\partial H}{\partial z^j}, \tag{1.4.2}$$

so the critical points of H, i.e. points where $\partial H/\partial z^j = 0$, correspond to steady-state solutions or equilibrium points of the system.

More is true in noncanonical Hamiltonian mechanics. Let C be a Casimir function, so that $\Pi^{ij}\partial C/\partial z^j = 0$. Then we can also write (1.4.1) as

$$\frac{dz^i}{dt} = \Pi^{ij}\frac{\partial}{\partial z^j}(H + C), \tag{1.4.3}$$

so the critical points of $A = H + C$ always correspond to equilibrium points of the noncanonical Hamiltonian system. The condition $\partial H/\partial z^j = -\partial C/\partial z^j$ for some Casimir function C is thus a sufficient condition for equilibrium. In particular, the gradient of the Hamiltonian H does not need to vanish provided that it can be cancelled by the gradient of a Casimir function. The method of identifying equilibria of a noncanonical Hamiltonian system from the critical points of a function $A = H + C$ is known as the *energy-Casimir method*. For applications in fluid dynamics and kinetic theory, the quantity $A = H + C$, which we also call the available energy, would become a functional of the field variables, and the critical points of A would be obtained from a variational principle. Casimir functionals are very common in applications in fluid dynamics and kinetic theory[6] – this in turn leads to many non-trivial equilibrium solutions to the continuum systems considered.

The variational principle obtained from the energy-Casimir method can sometimes lead to *nonlinear stability* results for the corresponding equilibria. In the finite-dimensional

[5]The Poisson tensor needs to satisfy an additional partial differential equation due to the Jacobi identity of the Poisson bracket – these notions are considered in detail in section **2.1.1**.

[6]See e.g. [94] for a comprehensive list of Casimir functionals in common noncanonical Hamiltonian systems.

example above, if the available energy A is a local minimum at the critical point z_e, or equivalently if the Hessian matrix

$$K_{ij} = \left.\frac{\partial^2 A}{\partial z^i \partial z^j}\right|_{z=z_e} \tag{1.4.4}$$

is positive definite[7], then the dynamics (1.4.2) near the equilibrium point $z = z_e$ is stable, since $A(z)$ is a constant of motion that also bounds the distance $|z - z_e|$ from the equilibrium point. Indeed, the earliest application of the energy-Casimir method in Arnold's work [7, 8, 9] is on the nonlinear stability of certain equilibria for incompressible fluids. These stability arguments are also compatible with the double bracket framework mentioned in section **1.3** – as long as A is non-increasing in time and bounds the distance from equilibrium $|z - z_e|$ suitably, a nonlinear stability result can be established.

The *energy-momentum* method is an extension of the energy-Casimir method for time-dependent solutions that evolve along a symmetry [124, 159, 163, 164]. The correspondence between one-parameter groups of symmetries and conserved quantities in ordinary Hamiltonian mechanics[8] is retained in noncanonical Hamiltonian mechanics. Again using our finite-dimensional example, if $J(z)$ is a conserved quantity of the Hamiltonian system (1.4.2), then $\{H, J\} = 0$, and hence $H(z)$ is invariant under the Hamiltonian flow generated by J:

$$\frac{dz^i}{d\epsilon} = \Pi^{ij}\frac{\partial J}{\partial z^j}, \tag{1.4.5}$$

where ϵ is the flow parameter. Let us denote the flow generated by (1.4.5) as $z \mapsto \phi_\epsilon^J(z)$, which is also the symmetry transformation generated by J. Now consider the *augmented available energy* $A = H + C - J$, where C is again a Casimir function. If z_w is a critical point of A, then

$$\left.\Pi^{ij}\frac{\partial H}{\partial z^j}\right|_{z=z_w} = \left.\Pi^{ij}\frac{\partial J}{\partial z^j}\right|_{z=z_w}, \tag{1.4.6}$$

so the time evolution for the point z_w under the Hamiltonian H is instantaneously described by the flow (1.4.5) of J. Moreover, since $\{A, J\} = 0$, the flow of J is also a symmetry of the augmented available energy A, so $\phi_\epsilon^J(z_w)$ is a critical point of A for all ϵ. Thus the problem $dz/dt = \{z, H\}, z(0) = z_w$ is solved by $z(t) = \phi_t^J(z_w)$, which means that z_w evolves along the symmetry generated by J.

[7] In infinite dimensions, one usually needs some coercivity as well as just positive-definiteness – see e.g. [7, 8, 9, 94] for more detail.

[8] This correspondence is known as *Noether's theorem* in Lagrangian mechanics.

In applications for three-dimensional continuum systems, we often require the energy to be translationally and rotationally invariant. In noncanonical Hamiltonian mechanics, we can express this in terms of the six conserved quantities $L_1, L_2, L_3, U_1, U_2, U_3$, where L_a is the a^{th} component of the total angular momentum, and U_a is the a^{th} component of the total linear momentum. We require L_a to generate rotations about the a^{th} axis and U_a to generate translations along the a^{th} axis. These quantities satisfy the following commutation relations[9]:

$$\{L_a, L_b\} = \epsilon_{abc} L_c, \quad \{L_a, U_b\} = \epsilon_{abc} U_c, \quad \{U_a, U_b\} = 0, \tag{1.4.7}$$

and of course that they are conserved: $\{L_a, H\} = \{U_a, H\} = 0$. Considering the augmented available energy functional $A = H + C - U_3$ in the energy-momentum method leads to *travelling wave* solutions that translate uniformly along the z-direction. Unlike linear waves, which have infinitesimal amplitude and require linearisation, these travelling waves obtained from the energy-momentum method are *exact, finite-amplitude* solutions to the noncanonical Hamiltonian system.

One well-known example of such finite-amplitude waves are nonlinear *Alfvén waves* in MHD [2, 3, 22, 194]. Consider the ideal incompressible MHD system. The fluid velocity $\mathbf{u}$ and magnetic field $\mathbf{B}$ evolve in time as

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \mathbf{B} \cdot \nabla \mathbf{B}, \qquad \nabla \cdot \mathbf{u} = 0, \tag{1.4.8a}$$

$$\partial_t \mathbf{B} + \mathbf{u} \cdot \nabla \mathbf{B} = \mathbf{B} \cdot \nabla \mathbf{u}, \qquad \nabla \cdot \mathbf{B} = 0, \tag{1.4.8b}$$

where P is the combined fluid and magnetic pressure, which enforces the incompressibility constraint $\nabla \cdot \mathbf{u} = 0$. The incompressible MHD system (1.4.8a,b) is well-known to be a noncanonical Hamiltonian system [6, 138]. Equations (1.4.8a,b) can also be written in terms of the *Elsässer variables* $\boldsymbol{\zeta}_\pm = \mathbf{u} \pm \mathbf{B}$ [22, 59] as

$$\partial_t \boldsymbol{\zeta}_\pm + \boldsymbol{\zeta}_\mp \cdot \nabla \boldsymbol{\zeta}_\pm = -\nabla P, \quad \nabla \cdot \boldsymbol{\zeta}_\pm = 0. \tag{1.4.9}$$

The cartesian components of $\boldsymbol{\zeta}_+$ are materially advected by $\boldsymbol{\zeta}_-$ and vice versa. The system (1.4.9) admits the following nonlinear Alfvén waves solutions:

$$\boldsymbol{\zeta}_+(\mathbf{x}, t) = \mathbf{w}, \quad \boldsymbol{\zeta}_-(\mathbf{x}, t) = \mathbf{a}(\mathbf{x} - \mathbf{w}t), \tag{1.4.10}$$

[9] Mathematically, we would like the quantities $L_1, L_2, L_3, U_1, U_2, U_3$ to be the components of a *moment map* $M \to (\mathfrak{so}(3) \ltimes \mathbb{R}^3)^*$, where $\mathfrak{so}(3) \ltimes \mathbb{R}^3$ is the Lie algebra for the three-dimensional Euclidean group $E(3) = SO(3) \ltimes \mathbb{R}^3$ of rigid body motions. Moment maps are discussed in section **2.5**.

where $\mathbf{w}$ is an arbitrary constant vector, and $\mathbf{a}(\mathbf{x})$ is an arbitrary divergence-free vector field. The nonlinear travelling wave solutions (1.4.10) are related to the critical points of the augmented available energy functional $A = H + C - J$ for

$$H = \int d^3x \, \frac{1}{2} \left(|\mathbf{u}|^2 + |\mathbf{B}|^2 \right), \quad C = \int d^3x \, \left(\mathbf{u} - \mathbf{w} \right) \cdot \mathbf{B}, \quad J = \int d^3x \, \mathbf{u} \cdot \mathbf{w}. \quad (1.4.11)$$

Indeed, requiring $\delta(H + C - J) = 0$ gives $\boldsymbol{\zeta}_+ = \mathbf{w}$ and $\boldsymbol{\zeta}_-$ arbitrary, which leads to the nonlinear Alfvén wave solutions (1.4.10) using the energy-momentum method.

We explore a new application of these principles in chapter **5**, where we formulate the dynamics of a fluid suspension of active, rod-like swimmers as a noncanonical Hamiltonian system. This formulation shares the same Poisson bracket with incompressible MHD, with a different expression for the Hamiltonian functional. As a result, the active rod system shares important Casimir functionals with MHD like *magnetic helicity* and *cross helicity* [94], which we exploit using the energy-Casimir and energy-momentum methods. In particular, the contractile (pulling) swimmers support nonlinear waves that we identify as the analogues of nonlinear Alfvén waves in MHD, and the static force-free equilibria of this active suspension obey variational principles analogous to static force-free MHD configurations [151, 169, 173, 191].

1.5 Hamiltonian reduction and hierarchical relationships between models

The noncanonical Hamiltonian framework can also be used to analyse the hierarchical relationship between different levels of description of the same physical system. The derivation of reduced Hamiltonian models from more primitive models is known as *Hamiltonian reduction*, and tools from Poisson geometry offers valuable insight in both studying existing reductions and discovering new reductions. Consider a primitive description of a physical system, which is a noncanonical Hamiltonian system formulated on the Poisson manifold M_1 and with Hamiltonian H_1. We would like to construct a reduced description of the same system, formulated on a possibly smaller configuration space M_2. The process of finding a reduced Hamiltonian system on M_2 can be broken down into the following steps:

1. Find a Poisson bracket on M_2.

2. Find a mathematical relationship between the Poisson brackets on M_1 and M_2.

3. Construct a reduced Hamiltonian H_2 on M_2 from H_1 using the mathematical relationship in step 2.

Typical mathematical relationships between the Poisson manifolds include being related by a Poisson map $J : M_1 \to M_2$ [84], or M_2 being a *Marsden–Weinstein quotient* of M_1 under some symmetry [123, 125, 130, 131]. We discuss these possibilities in section **2.5**.

In many cases, obtaining the reduced Hamiltonian H_2 involves making some uncontrolled approximations in the primitive Hamiltonian H_1, such as ignoring some formally small terms or imposing some constraints. On the surface, this is no better or worse than making these approximations directly in the equations of motion – in chaotic systems, the neglected small terms act as small sources of error that accumulate over time, so the solutions of the reduced system do not stay close to those of the primitive system, except perhaps in some statistical sense. However, by making these approximations in a Hamiltonian way, the reduced system can be made to possess desirable *structural properties*, such as exact conservation laws for the approximated forms of physical quantities, or symmetries inherited from the primitive system[10]. Formulating the reduced system as a noncanonical Hamiltonian system also permits us to use the energy-Casimir and energy-momentum methods to study its solutions (see section **1.4**), although the relationship between the respective spaces of Casimir functionals on M_1 and M_2 is not always straightforward.

These approximate Hamiltonian reductions are very common in kinetic theory and mathematical physics. In semiclassical mechanics, the Hamilton–Jacobi equation can be obtained from the Schrödinger equation by first performing the Madelung transform and then taking the classical limit $\hbar \to 0$ in the Hamiltonian functional [105, 106]. In kinetic theory, the Vlasov–Poisson equation can be derived from the BBGKY hierarchy by substituting the ansatz $f_2 = f_1 f_1$ in the Hamiltonian functional [126]. In plasma physics, Hamiltonian fluid models of drift kinetics are found in [170, 171, 172], where the reduced Poisson bracket is obtained by imposing constraints on the primitive Poisson bracket.

The equivalent procedure in Lagrangian mechanics, where approximations are made directly in the variational principle, is also extensively used in fluid dynamics and the theory of nonlinear waves. In shallow water theory, the shallow water and Green–Naghdi equations can be derived by imposing constraints on columnar motion in the variational principle for general ideal incompressible fluids [132]. In geophysical fluid dynamics, the small Rossby number approximation can be made in the variational principle to derive manifestly conservative equations for nearly geostrophic flow [152]. In the theory of modulated waves, where waves propagate in a slowly varying media, the Whitham modulation equations can be derived by averaging the fast scales in the variational principle [185, 186, 187]. Similarly, in nonlinear optics, the particle-like reduced dynamics of solitons in the discrete nonlinear

[10]This point is thoughtfully discussed in [152], pages 473–474.

Schrödinger equation can be obtained by making an ansatz in the variational principle [104, 120].

Hamiltonian reduction can also be used to identify special solutions of a Hamiltonian system on M_1. This is achieved by considering a Poisson map $I : M_2 \to M_1$ from a smaller Poisson manifold M_2 into M_1 and by restricting the dynamics on the image $I(M_2)$. For example, an extended model of MHD that accounts for the Hall effect is formulated as a noncanonical Hamiltonian system in [1]. There is a Poisson manifold corresponding to configurations that are translationally invariant along the z-axis [102]. In kinetic theory, the one-dimensional waterbag reduction of the Benney hydrodynamic chain [15, 39, 195] and the cold plasma reduction of the Vlasov–Poisson equation [70, 72, 73, 176, 177] are examples of such special solutions that we will discuss further in section **4.5**.

As an application of these principles, we consider the Hamiltonian reduction of gas kinetic theory to hydrodynamics in chapter **4**, based on the author's work [42]. At the beginning of this chapter, we considered the Chapman–Enskog expansion in gas kinetic theory, which is an asymptotic derivation of the compressible Euler and Navier–Stokes–Fourier equations (1.1.1a-c) from the linearised Boltzmann equation (1.1.4) in the strongly collisional limit $\mathrm{Kn} \to 0$. The Chapman–Enskog expansion thus provides an asymptotic justification of the physical validity of the macroscopic hydrodynamic descriptions (1.1.1a-c) as reduced models for kinetic theory. Curiously, the *collisionless Boltzmann equation*, i.e. the Boltzmann equation (1.1.4) without the collision term on the right-hand side, is also a noncanonical Hamiltonian system [71, 130]. The full Boltzmann equation is of course not Hamiltonian, as the collision operator $C[f, f]$ introduces time-irreversibility. Yet the compressible Euler equations, derived as an asymptotic limit of the Boltzmann equation for strong collisions, form a noncanonical Hamiltonian system [94, 138]. This invites the question of whether we can obtain hydrodynamics from kinetic theory by making the approximation $f \simeq f_m$ in a way that respects the Hamiltonian structure in both systems, which we answer affirmatively in chapter **4**. We construct a Poisson map from distribution functions to hydrodynamic variables. By making the ansatz $f \simeq f_m$ in the kinetic-theory Hamiltonian, we obtain an approximate Hamiltonian reduction from the collisionless Boltzmann equation to the compressible Euler equations.

Chapter 2

The mathematics of noncanonical Hamiltonian mechanics

In this chapter we review the foundational material on noncanonical Hamiltonian mechanics and indicate some of its well-known applications. In section **2.1**, we recall the notions of a Poisson manifold and a Poisson algebra. We indicate our formal[1] approach to infinite-dimensional Poisson manifolds, and introduce the important concept of an *affine Poisson bracket* on a vector space. Affine Poisson brackets, which are found in many applications, appear naturally on the dual spaces to Lie algebras. In section **2.2**, we review some key constructions in the theory of Lie algebras, such as the *semidirect product* and the *central extension*. In section **2.3** we give some examples of infinite-dimensional Lie algebras from differential geometry. Each of these Lie algebras is a space of sections of a naturally constructed vector bundle over a finite-dimensional manifold.

With the aforementioned examples in mind, we introduce noncanonical Hamiltonian mechanics properly in section **2.4**. We discuss the idea of *available energy* in a noncanonical Hamiltonian system, and indicate its connections with nonlinear stability and non-equilibrium thermodynamics. In section **2.5** we consider the problem of *reduction* in noncanonical Hamiltonian mechanics, where one seeks a reduced description of a more primitive noncanonical Hamiltonian system. There are many ways that such reductions can be carried out; the main methods are reduction via a *Poisson map* and *Marsden–Weinstein reduction* using a symmetry. Finally, we give some examples of common noncanonical Hamiltonian systems in fluid dynamics and kinetic theory in section **2.6**.

The author claims no originality to the results in this chapter. The main references are given at the beginning of each section.

[1] By "formal" we mean that we forgo a careful treatment of analytical issues and instead focus on algebraic aspects.

2.1 Poisson structures

In this section we recall the notions of a Poisson manifold and a Poisson algebra. We indicate the formal approach taken with infinite-dimensional Poisson manifolds, and give the affine Poisson bracket as an important example. The main references are [28, 107, 114, 183].

2.1.1 Finite-dimensional Poisson manifolds

Let M be a finite-dimensional manifold. A *Poisson bracket* on M is a bilinear skew-symmetric map $\{\cdot,\cdot\} : C^\infty(M) \times C^\infty(M) \to C^\infty(M)$ that satisfies the Leibniz and Jacobi identities:

$$\{f, gh\} = \{f, g\}h + g\{f, h\}, \tag{2.1.1a}$$

$$\{\{f, g\}, h\} + \{\{g, h\}, f\} + \{\{h, f\}, g\} = 0, \tag{2.1.1b}$$

for any $f, g, h \in C^\infty(M)$. The manifold M is then called a *Poisson manifold*. Since the Leibniz identity (2.1.1a) holds, the Poisson bracket $\{f, g\}$ depends bilinearly on df and dg. We can thus express the Poisson bracket in terms of a skew-symmetric second rank contravariant tensor $\Pi \in \Gamma(\wedge^2 TM)$, called the *Poisson tensor*, defined by

$$\{f, g\} = \Pi(df, dg), \tag{2.1.2}$$

for any $f, g, \in C^\infty(M)$. In particular, if $y(x)$ is a single-variable real function, then

$$\{y(f), g\} = y'(f)\{f, g\}. \tag{2.1.3}$$

Let us investigate the Jacobi identity (2.1.1b) in more detail. Define the *Jacobinator* $Jac_\Pi : C^\infty(M) \times C^\infty(M) \times C^\infty(M) \to C^\infty(M)$ of Π to be the skew-symmetric trilinear map

$$Jac_\Pi(f, g, h) := \{\{f, g\}, h\} + \{\{g, h\}, f\} + \{\{h, f\}, g\}, \tag{2.1.4}$$

for any $f, g, h \in C^\infty(M)$. The Jacobinator satisfies the Leibniz identity

$$Jac_\Pi(f, g, hk) = Jac_\Pi(f, g, h)k + hJac_\Pi(f, g, k), \tag{2.1.5}$$

so $Jac_\Pi(f, g, h)$ depends trilinearly on df, dg, dh. Thus we can identify it with a tensor $Jac_\Pi \in \Gamma(\wedge^3 TM)$. The Jacobi identity (2.1.1b) is now equivalent to the vanishing of Jac_Π. In local coordinates z^i, this condition is

$$(Jac_\Pi)^{ijk} := \Pi^{il}\frac{\partial \Pi^{jk}}{\partial z^l} + \Pi^{jl}\frac{\partial \Pi^{ki}}{\partial z^l} + \Pi^{kl}\frac{\partial \Pi^{ij}}{\partial z^l} = 0, \tag{2.1.6}$$

so we can equivalently express the Jacobi identity (2.1.1b) as a system of partial differential equations on the components Π^{ij}.

The *rank* of the Poisson tensor at a point $z \in M$ is the rank of the matrix $\Pi^{ij}(z)$. When the rank of Π is equal to $\dim(M)$ everywhere, M is called a *symplectic manifold*. This agrees with the more conventional definition, where a symplectic manifold is defined as a manifold M equipped with a non-degenerate, closed 2-form ω. If we are given either a Poisson tensor Π of full rank or a non-degenerate 2-form ω, we can define the other by the equation $\omega_{ij}\Pi^{jk} = -\delta_i^k$. The identity

$$\Pi^{im}\Pi^{ln}\Pi^{jk}\frac{\partial \omega_{ij}}{\partial z^l} = -\Pi^{ln}\frac{\partial \Pi^{jk}}{\partial z^l} \tag{2.1.7}$$

then implies that ω is closed if and only if Π satisfies (2.1.6).

The local theory of Poisson manifolds is extensively studied in [183]. The key result is the *Weinstein splitting theorem*:

Theorem 2.1 (Weinstein)**.** *Let M be a finite-dimensional Poisson manifold. At any $z \in M$, there exists a set of local coordinates $q_1, \dots q_m, p_1, \dots p_m, y_1, \dots y_l$, where $2m + l = \dim(M)$, such that*

$$\Pi = \sum_{i=1}^{m} \frac{\partial}{\partial q_i} \wedge \frac{\partial}{\partial p_i} + \sum_{i,j=1}^{l} \frac{1}{2}\psi_{ij}(y_1, \dots, y_l)\frac{\partial}{\partial y_i} \wedge \frac{\partial}{\partial y_j}, \tag{2.1.8}$$

where $\psi_{ij}(y)$ is an antisymmetric matrix of functions that tend to zero as $|y| \to 0$.

The coordinates $q_1, \dots, q_m, p_1, \dots, p_m, y_1, \dots, y_l$ are known as *Darboux coordinates*. The surface locally parametrised by $y_1 = \dots = y_l = 0$ is called the *symplectic leaf through* z. One can always find a maximal connected symplectic leaf S_z through z by taking the union of these $y_1 = \dots = y_l = 0$ surfaces constructed through the use of Darboux coordinates, as z varies along the surface. A maximal connected symplectic leaf is often simply referred to as a symplectic leaf. The tangent space to the symplectic leaf is precisely the image of $\Pi : T_z^*M \to T_zM$. Any finite-dimensional Poisson manifold is a union of symplectic leaves. In particular, if M is a symplectic manifold, then the expression for Π in Darboux coordinates is $\sum_{i=1}^{m}(\partial/\partial q_i) \wedge (\partial/\partial p_i)$, and the only symplectic leaf is the connected components of M.

A point $z \in M$ is a *regular point* if the rank of Π is locally constant at z, or equivalently that the functions $\psi_{ij}(y)$ vanish identically in a set of Darboux coordinates around z. The set of regular points is open and dense in M. Any sufficiently small neighbourhood U of a regular point z can be foliated by symplectic leaves of the same dimension $2m$, defined in Darboux coordinates as the loci $y_1 = \lambda_1, \dots, y_l = \lambda_l$ where $\lambda_1, \dots, \lambda_l$ are constants.

2.1.2 Poisson algebras and Poisson maps

Let A be an associative commutative algebra over $\mathbb{R}$. We denote the associative commutative operation by juxtaposition $(f, g) \mapsto fg$ and call it multiplication. The commutative algebra A is called a *Poisson algebra* if we have an additional bilinear skew-symmetric map $\{\cdot, \cdot\} : A \times A \to A$, called the Poisson bracket, that satisfies the Leibniz identity (2.1.1a) with respect to multiplication on A and the Jacobi identity (2.1.1a). The main example of a Poisson algebra is the space of smooth functions on a Poisson manifold M.

A *Poisson subalgebra* S of A is a subspace that is closed under both multiplication and Poisson brackets: $SS \subset S, \{S, S\} \subset S$. A *Poisson ideal* I of A is a subspace that is an ideal for both multiplication and the Poisson bracket: $AI \subset I, \{A, I\} \subset I$.

Let A_1 and A_2 be Poisson algebras, with Poisson brackets $\{\cdot, \cdot\}_1$ and $\{\cdot, \cdot\}_2$ respectively. A *Poisson algebra morphism* $\phi : A_1 \to A_2$ is a linear map that satisfies

$$\phi(f)\phi(g) = \phi(fg), \tag{2.1.9a}$$

$$\{\phi(f), \phi(g)\}_2 = \phi\left(\{f, g\}_1\right), \tag{2.1.9b}$$

for all $f, g \in A_1$. A map $J : M_2 \to M_1$ is called a *Poisson map* if its pullback on functions $J^* : C^\infty(M_1) \to C^\infty(M_2)$ is a Poisson algebra morphism. The pullback of any map $M_2 \to M_1$ trivially satisfies (2.1.9a), so (2.1.9b) is the only condition that needs checking. If the Poisson map $J : M_2 \to M_1$ is also an embedding, we identify M_2 with its image $J(M_2)$ and call it a *Poisson submanifold*.

If S is a Poisson subalgebra of the Poisson algebra A, then the inclusion $S \hookrightarrow A$ is a Poisson algebra morphism. If I is a Poisson ideal of A, the quotient vector space A/I is endowed with a canonical Poisson algebra structure for which the quotient map $A \to A/I$ is a Poisson algebra morphism.

Given a Poisson algebra A, there is an important subalgebra $Cas(A)$ called the space of *Casimir elements* of A, defined as

$$Cas(A) := \{C \in A : \{C, f\} = 0 \text{ for all } f \in A\} \tag{2.1.10}$$

The Poisson algebra A can thus be regarded as a $Cas(A)$-module, in the sense that any $C \in Cas(A)$ behaves like a scalar with respect to both multiplication and the Poisson bracket. If A is the algebra of functions on a Poisson manifold M, then we also call the Casimir elements *Casimir function(al)s* and denote the space of Casimir functions by $Cas(M)$. An alternative characterisation for $Cas(M)$ can be given in terms of the Poisson tensor:

$$Cas(M) = \{C \in C^\infty(M) : \Pi(\alpha, dC) = 0 \text{ for all } z \in M \text{ and all } \alpha \in T_z^*M\}. \tag{2.1.11}$$

Thus $Cas(M)$ is precisely the space of functions that are constant on the symplectic leaves. In a small neighbourhood U of a regular point $z \in M$ with Darboux coordinates $q_1, \ldots, q_m, p_1, \ldots p_m, y_1, \ldots, y_l$, the space $Cas(U)$ is the algebra of functions on $y_1, \ldots, y_l$. The zero locus $C = 0$ of a Casimir function C is always a Poisson submanifold if it is a manifold. The algebra of functions on $C = 0$ is then $C^\infty(M)/\langle C \rangle$, where $\langle C \rangle$ is the multiplicative ideal generated by C, which is always a Poisson ideal because C is a Casimir function.

2.1.3 Infinite-dimensional vector spaces

Let V be a Banach space or a Fréchet space, not necessarily finite-dimensional. In the applications we are concerned with later, V is typically a space of (smooth) functions over a finite-dimensional manifold, or more generally a space of (smooth) sections of a finite-rank vector bundle over a finite-dimensional manifold, in which case we call V a space of *fields*. Let $\mathcal{F}(V)$ denote a space of suitable functionals on V. A *Poisson bracket* on V is a bilinear skew-symmetric operation $\{\cdot, \cdot\} : \mathcal{F}(V) \times \mathcal{F}(V) \to \mathcal{F}(V)$ that satisfies the Leibniz (2.1.1a) and Jacobi (2.1.1b) identities. While the formulation is identical to that in finite dimensions, there are some analytical issues unique to infinite dimensions. One possible resolution is to restrict our attention to sufficiently regular functionals, as we shall illustrate.

Given a sufficiently regular functional $F[z]$, we can define a V^*-valued functional called its *functional derivative* $\delta F/\delta z : V \to V^*$ by

$$\left\langle \frac{\delta F}{\delta z}[z], v \right\rangle = \lim_{\epsilon \to 0} \frac{F[z + \epsilon v] - F[z]}{\epsilon}, \tag{2.1.12}$$

for any v in V, where the angle brackets denote the dual pairing between V and V^*. Functional derivatives of vector-valued functionals is defined similarly, whenever the right-hand side of (2.1.12) is unambiguously defined. The second derivative is defined as the functional derivative of the V^*-valued functional $\delta F/\delta z : V \to V^*$, and similarly for higher order functional derivatives. We can formulate the *functional chain rule* with this definition of the functional derivative. Let V, W be vector spaces, and $T : V \to W$ be a sufficiently regular W-valued functional on V. If $F : W \to \mathbb{R}$ is a sufficiently regular functional on W, then its pullback $T^*F = W \circ T$ defines a functional on V. The functional derivative of T^*F is

$$\begin{aligned} \lim_{\epsilon \to 0} \frac{T^*F[z + \epsilon v] - T^*F[v]}{\epsilon} &= \left\langle \frac{\delta T^*F}{\delta z}[z], v \right\rangle \\ = \left\langle \frac{\delta F}{\delta w}\left[T[z]\right], \frac{\delta T}{\delta z}[z]v \right\rangle &= \left\langle \left(\frac{\delta T}{\delta z}[z]\right)^* \frac{\delta F}{\delta w}\left[T[z]\right], v \right\rangle, \end{aligned} \tag{2.1.13}$$

where $z, v \in V$, and $(\delta T/\delta z)^*[z]$ is the formal linear adjoint of $(\delta T/\delta z)[z] : V \to W$ at a particular z.

As an application of these ideas, consider the graph of the map $T : V \to W$ in $V \times W$. Denote the inclusion map of the graph by $\iota : V \to V \times W$, defined explicitly as $\iota[v] = (v, T[v])$ for $v \in V$. Also define the projection map to the first factor $\pi : V \times W \to V$ given by $\pi[v, w] = v$ for all $v \in V$ and all $w \in W$. If F is a functional on V, then the functional derivative of $\pi^* F : V \times W \to \mathbb{R}$ is

$$\left(\frac{\delta \pi^* F}{\delta v}[v, w], \frac{\delta \pi^* F}{\delta w}[v, w]\right) = \left(\frac{\delta F}{\delta v}[v], 0\right), \tag{2.1.14}$$

for all $v \in V$ and all $w \in W$. Meanwhile, if G is a functional on $V \times W$, the functional derivative of $\iota^* G : V \to \mathbb{R}$ is

$$\frac{\delta \iota^* G}{\delta v}[v] = \frac{\delta G}{\delta v}[v, T[v]] + \left(\frac{\delta T}{\delta v}[v]\right)^* \frac{\delta G}{\delta w}[v, T[v]], \tag{2.1.15}$$

for all $v \in V$. While $\pi\iota : V \to V$ is the identity map, the map $\iota\pi : V \times W \to V \times W$ depends on the map $T : V \to W$ in general, and

$$\left(\frac{\delta \pi^* \iota^* G}{\delta v}[v, w], \frac{\delta \pi^* \iota^* G}{\delta w}[v, w]\right) = \left(\frac{\delta G}{\delta v}[v, 0] + \left(\frac{\delta T}{\delta v}[v]\right)^* \frac{\delta G}{\delta w}[v, T[v]], 0\right), \tag{2.1.16}$$

where $G : V \times W \to \mathbb{R}$ is a sufficiently regular functional.

Let us return to Poisson brackets. Suppose that we have a sufficiently regular Poisson bracket on V, so that we can write it in terms of a Poisson tensor $\Pi[z]$, which is a smoothly varying skew-symmetric bilinear form $V^* \times V^* \to \mathbb{R}$ defined by the relation

$$\{F, G\}[z] = \Pi[z]\left(\frac{\delta F}{\delta z}[z], \frac{\delta G}{\delta z}[z]\right), \tag{2.1.17}$$

for all $F, G \in \mathcal{F}(V)$. This naive definition is problematic however, because the domain of $\Pi[z]$ is not all of $V^* \times V^*$ in many applications. For example, let $V = C^\infty(S^1)$, where S^1 is the unit circle with coordinate θ, with typical element $z(\theta) \in V$, and consider the following Poisson bracket

$$\{F, G\} = \int_0^{2\pi} d\theta \; z(\theta)\left(\frac{\delta F}{\delta z}\frac{\partial}{\partial \theta}\frac{\delta G}{\delta z} - \frac{\delta G}{\delta z}\frac{\partial}{\partial \theta}\frac{\delta F}{\delta z}\right). \tag{2.1.18}$$

The full continuous dual V^* would contain distributions on S^1. If $\delta F/\delta z$ and $\delta G/\delta z$ are both distributions, then $\{F, G\}$ would be ill-defined. To circumvent this issue, we choose to work with "smooth duals". A *smooth dual* V_s^* to a vector space V is a subspace of the full continuous dual V^* that has a weakly non-degenerate pairing with V, which means that

$$\langle \alpha, v \rangle = 0 \text{ for all } \alpha \in V_s^* \Rightarrow v = 0, \tag{2.1.19a}$$

$$\langle \alpha, v \rangle = 0 \text{ for all } v \in V \Rightarrow \alpha = 0. \tag{2.1.19b}$$

The choice of a smooth dual is not unique and is usually motivated by context. For example, for $V = C^\infty(S^1)$, we can choose $V_s^* = C^\infty(S^1)$ with the dual pairing given by integration on S^1. If we take $\mathcal{F}(V)$ to be the space of functionals whose functional derivatives take values in V_s^*, then the expression (2.1.18) is well-defined for $F, G \in \mathcal{F}(V)$, and moreover $\{F, G\} \in \mathcal{F}(V)$, so that $\mathcal{F}(V)$ is a Poisson algebra. The issue of $V \subsetneq V^{**}$ for non-reflexive infinite-dimensional vector spaces can also be sidestepped in this setting, because we can always take V to be the smooth dual of V_s^*. We will henceforth omit the subscript s from the notation, so that V^* always denotes the smooth dual of V in the following.

Remark 2.1. There are settings in which some Banach space methods can be retained. We could have taken the space V to be a Sobolev space $H^s(S^1)$, with $s > 1 + 1/2$, and declare "sufficiently regular functionals" to be smooth functionals F whose functional derivatives take values in V, in the sense that $\delta F/\delta z$ is in the image of the canonical embedding $V \subset L^2(S^1) \subset V^*$, and similarly for higher derivatives. The expression $\{F, G\}$ (2.1.18) is then a well-defined functional on V. This amounts to choosing the smooth dual of $V = H^s(S^1)$ as $H^s(S^1)$, with the L^2-inner product as the weakly non-degenerate pairing.

Remark 2.2. Some authors do not work under our setting and instead allow functionals whose functional derivatives are distributional, such as $F[z] = \int d\theta\ z(\theta)\delta(\theta - \theta_0)$, and only require the Leibniz and Jacobi identities (2.1.1a,b) for the Poisson bracket to be satisfied when the expressions are well-defined. The main advantage of our approach is that, while we have merely sidestepped the analytical issues, the resulting space of sufficiently regular functionals $\mathcal{F}(V)$ is a Poisson algebra. We can then make mathematically rigorous statements in an algebraic sense.

The *affine Poisson brackets* on a vector space V, where the Poisson tensor $\Pi[z]$ is an affine function of $z \in V$, constitute an important class of examples of infinite-dimensional Poisson manifolds. The explicit expression of the Poisson tensor for an affine Poisson bracket is

$$\Pi(z)(\alpha, \beta) = \langle c(\alpha, \beta), z\rangle + \Omega(\alpha, \beta), \tag{2.1.20}$$

where $c : V^* \times V^* \to V^*$ is a skew-symmetric V^*-valued bilinear form, and $\Omega : V^* \times V^* \to \mathbb{R}$ is a skew-symmetric bilinear form. A lengthy direct computation [30] shows that the Jacobinator of Π is

$$\begin{aligned} Jac_\Pi(F, G, H) = &\left\langle z, c\left(c\left(\frac{\delta F}{\delta z}, \frac{\delta G}{\delta z}\right), \frac{\delta H}{\delta z}\right)\right\rangle + \Omega\left(c\left(\frac{\delta F}{\delta z}, \frac{\delta G}{\delta z}\right), \frac{\delta H}{\delta z}\right) \\ &+ \left\langle z, c\left(c\left(\frac{\delta G}{\delta z}, \frac{\delta H}{\delta z}\right), \frac{\delta F}{\delta z}\right)\right\rangle + \Omega\left(c\left(\frac{\delta G}{\delta z}, \frac{\delta H}{\delta z}\right), \frac{\delta F}{\delta z}\right) \\ &+ \left\langle z, c\left(c\left(\frac{\delta H}{\delta z}, \frac{\delta F}{\delta z}\right), \frac{\delta G}{\delta z}\right)\right\rangle + \Omega\left(c\left(\frac{\delta H}{\delta z}, \frac{\delta F}{\delta z}\right), \frac{\delta G}{\delta z}\right), \end{aligned} \tag{2.1.21}$$

as long as the second functional derivatives of F, G, H are well-defined and symmetric: $\delta^2 F/\delta z \delta z' = \delta^2 F/\delta z' \delta z$, and similarly for G, H. The Jacobinator Jac_Π vanishes for all z precisely when $c : V^* \times V^* \to V^*$ endows V^* with the structure of a *Lie algebra*, and when $\Omega : V^* \times V^* \to \mathbb{R}$ is a 2-*cocycle* of this Lie algebra. We will discuss Lie algebras and cocycles in much greater detail in section **2.2**. Conversely, given a Lie algebra structure c on V^* and a 2-cocycle Ω for this Lie algebra, the formula (2.1.20) defines an affine Poisson bracket on V.

As an example, consider the case where $c = 0$ in (2.1.20). The Jacobi identity is then automatically satisfied for any choice of Ω. These Poisson brackets are called *constant Poisson brackets*. An important special case is when $V = W \times W^*$ for some other vector space W. Such V is called a *symplectic vector space*, and there is a canonical weakly non-degenerate skew-symmetric bilinear form called the *symplectic form* defined by the formula

$$\omega\left((w_1, \alpha_1), (w_2, \alpha_2)\right) := \langle \alpha_2, w_1 \rangle - \langle \alpha_1, w_2 \rangle, \tag{2.1.22}$$

where $w_1, w_2 \in W$ and $\alpha_1, \alpha_2 \in W^*$. The constant Poisson bracket on $\mathcal{F}(W \times W^*)$ is then

$$\{F, G\}[w, \alpha] = \left\langle \frac{\delta F}{\delta w}, \frac{\delta G}{\delta \alpha} \right\rangle - \left\langle \frac{\delta G}{\delta w}, \frac{\delta F}{\delta \alpha} \right\rangle, \tag{2.1.23}$$

where $F, G \in \mathcal{F}(W \times W^*)$.

2.1.4 The algebraic approach to affine Poisson brackets

There is an algebraic alternative to the formal approach to functionals considered in section **2.1.3**, which is more restrictive in scope but can be treated with more mathematical rigour. Let W be a vector space, and consider the algebra $\mathcal{P}ol(W)$ of commuting polynomials generated by the monomials $\alpha \in W$. $\mathcal{P}ol(W)$ is sometimes called the *symmetric algebra* of W.

Now consider a Poisson bracket $\{\cdot, \cdot\} : \mathcal{P}ol(W) \times \mathcal{P}ol(W) \to \mathcal{P}ol(W)$ on $\mathcal{P}ol(W)$. The Leibniz identity (2.1.1a) then dictates that the Poisson bracket is zero on constants and is completely determined by its values on the monomials $\alpha \in W$.

Now let us consider affine Poisson brackets on $\mathcal{P}ol(W)$. On the generators $\alpha, \beta \in W$, any affine Poisson bracket takes the form

$$\{\alpha, \beta\} = c(\alpha, \beta) + \Omega(\alpha, \beta), \tag{2.1.24}$$

where $c : W \times W \to W$ is a skew-symmetric W-valued bilinear form, and $\Omega : W \times W \to \mathbb{R}$ is a skew-symmetric bilinear form. The Jacobi identity (2.1.1b) is now equivalent to requiring

$$\{\{\alpha, \beta\}, \gamma\} + \{\{\beta, \gamma\}, \alpha\} + \{\{\gamma, \alpha\}, \beta\} = 0, \tag{2.1.25}$$

for all $\alpha, \beta, \gamma \in W$. Computing one of the terms in (2.1.25) gives

$$\{\{\alpha, \beta\}, \gamma\} = \{c(\alpha, \beta), \gamma\} + \{\Omega(\alpha, \beta), \gamma\} = c(c(\alpha, \beta), \gamma) + \Omega(c(\alpha, \beta), \gamma), \tag{2.1.26}$$

so taking cyclic permutations and summing gives the two identities at degrees 1 and 0 respectively:

$$c(c(\alpha, \beta), \gamma) + c(c(\beta, \gamma), \alpha) + c(c(\gamma, \alpha), \beta) = 0, \tag{2.1.27a}$$

$$\Omega(c(\alpha, \beta), \gamma) + \Omega(c(\beta, \gamma), \alpha) + \Omega(c(\gamma, \alpha), \beta) = 0, \tag{2.1.27b}$$

which again states that c endows W with the structure of a Lie algebra, and that Ω is a 2-cocycle on this Lie algebra[2].

This formulation of affine Poisson bracket is purely algebraic and makes no reference to any additional structure that the vector space W may possess, such as a topology or a norm. The relationship between this algebraic approach and the approach given in section **2.1.3** is that the vector space W should be thought of as the smooth dual space to the affine Poisson manifold V considered previously, and that the polynomials on $W = V^*$ should be thought of as polynomial functionals on V. In this setting, the algebra of suitable functionals $\mathcal{F}(V)$ on V is no smaller (and typically strictly larger) than the polynomial algebra $\mathcal{P}ol(W)$. For example, if V is finite-dimensional, then $\mathcal{F}(V) = C^\infty(V)$, which includes polynomial functions as well as transcendental functions. The algebraic approach is more restrictive on the types of functionals that one is allowed to consider, but offers a path to rigorous mathematical results when one has not prepared a fully analytical theory of functionals for the particular application.

2.2 Lie algebras and affine Poisson brackets

We have shown in section **2.1.3** that there is a one-to-one correspondence between affine Poisson brackets on a vector space V and the data (c, Ω) on its smooth dual V^*, where $c : V^* \times V^* \to V^*$ is a Lie algebra operation and $\Omega : V^* \times V^* \to \mathbb{R}$ is a 2-cocycle for the Lie algebra. The study of affine Poisson brackets, many of which are of interest in applications, is then equivalent to the study of Lie algebras and their 2-cocycles. This section discusses some common constructions related to Lie algebras and their 2-cocycles.

[2]We discuss Lie algebras and cocycles in greater detail in section **2.2**.

2.2.1 Definitions

A *Lie algebra* $\mathfrak{g}$ is a vector space with a skew-symmetric bilinear operation $[\cdot,\cdot] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ that satisfies the Jacobi identity:

$$[[X,Y],Z] + [[Y,Z],X] + [[Z,X],Y] = 0. \tag{2.2.1}$$

The operation $[\cdot,\cdot]$ is commonly called the *Lie bracket*. A *Lie subalgebra* $\mathfrak{h}$ is a vector subspace of $\mathfrak{g}$ that is closed under the Lie bracket: $[\mathfrak{h},\mathfrak{h}] \subset \mathfrak{h}$. A *Lie ideal* (or simply *ideal*) I is a vector subspace of $\mathfrak{g}$ that satisfies $[\mathfrak{g}, I] \subset I$. The *centre* $Z(\mathfrak{g})$ of a Lie algebra is the Lie subalgebra

$$Z(\mathfrak{g}) := \{X \in \mathfrak{g} : [X,Y] = 0 \text{ for all } Y \in \mathfrak{g}\}. \tag{2.2.2}$$

A Lie algebra is called *abelian* if $Z(\mathfrak{g}) = \mathfrak{g}$, or equivalently if the Lie bracket operation is identically zero. The *commutator ideal* $[\mathfrak{g},\mathfrak{g}]$ is the Lie ideal

$$[\mathfrak{g},\mathfrak{g}] := \{[X,Y] : X, Y \in \mathfrak{g}\}. \tag{2.2.3}$$

A Lie algebra is called *perfect* if $[\mathfrak{g},\mathfrak{g}] = \mathfrak{g}$.

A *Lie algebra homomorphism* $\phi : \mathfrak{g}_1 \to \mathfrak{g}_2$ from the Lie algebra $\mathfrak{g}_1$ to the Lie algebra $\mathfrak{g}_2$ is a linear map that satisfies

$$[\phi(X), \phi(Y)]_2 = \phi\left([X,Y]_1\right), \tag{2.2.4}$$

for all $X, Y \in \mathfrak{g}_1$, where $[\cdot,\cdot]_1$ denotes the Lie bracket on $\mathfrak{g}_1$ and similarly for $\mathfrak{g}_2$. An *isomorphism* of Lie algebras is an invertible Lie algebra homomorphism whose inverse is also a Lie algebra homomorphism. The inclusion map of a Lie subalgebra $\mathfrak{h} \hookrightarrow \mathfrak{g}$ is a Lie algebra homomorphism. The quotient vector space $\mathfrak{g}/I$ for $I \subset \mathfrak{g}$ a Lie ideal can be given a canonical Lie algebra structure such that the quotient map $\mathfrak{g} \to \mathfrak{g}/I$ is a Lie algebra homomorphism.

Let V be a vector space. The space $End(V)$ of linear endomorphisms $T : V \to V$ is a Lie algebra, with the Lie bracket given by the commutator $[T_1, T_2] = T_1T_2 - T_2T_1$. A *representation* of a Lie algebra $\mathfrak{g}$ on V is then defined as a Lie algebra homomorphism $\phi : \mathfrak{g} \to End(V)$. We write the action of $\mathfrak{g}$ on V by this representation as $X \cdot v = \phi(X)v$ for $X \in \mathfrak{g}$ and $v \in V$.

A Lie algebra $\mathfrak{g}$ always have a representation on itself, called the *adjoint representation* $ad : \mathfrak{g} \to End(\mathfrak{g})$ defined by $X \mapsto [X,\cdot]$. The Jacobi identity (2.2.1) ensures that the linear map ad defines a representation.

Let V be a representation of $\mathfrak{g}$. We can define a representation of $\mathfrak{g}$ on the smooth dual V^* of V, called the *dual representation* of V, where the action of $\mathfrak{g}$ on V^* is the negative of the formal linear adjoint of that on V:

$$\langle X \cdot \alpha, v \rangle = -\langle \alpha, X \cdot v \rangle, \tag{2.2.5}$$

where $\alpha \in V^*$ and $v \in V$. The dual representation of the adjoint representation is called the *coadjoint representation*.

Let $W \subset V$ be a linear subspace of the representation V. The subspace W is called an *invariant subspace* if W is fixed by the $\mathfrak{g}$-action: $X \cdot w \in W$ for any $X \in \mathfrak{g}$ and any $w \in W$. Restricting the $\mathfrak{g}$-action on V to W then makes W into a representation of $\mathfrak{g}$, which we call a *subrepresentation*. The quotient vector space V/W for W an invariant subspace of V also inherits a well-defined $\mathfrak{g}$-action that makes it into a representation of $\mathfrak{g}$; this is called the *quotient representation*.

Let $\mathfrak{g}$ be a Lie algebra, and $\mathfrak{g}^*$ be its smooth dual. We denote a typical element of $\mathfrak{g}^*$ by m. The space $\mathcal{F}(\mathfrak{g}^*)$ of sufficiently regular functionals on $\mathfrak{g}^*$ can be made into a Poisson algebra by equipping it with the $(\pm)$-*Lie–Poisson bracket*

$$\{F, G\}_{\mathfrak{g}}[m] := \pm \left\langle m, \left[\frac{\delta F}{\delta m}, \frac{\delta G}{\delta m} \right] \right\rangle, \tag{2.2.6}$$

where $F, G \in \mathcal{F}(\mathfrak{g}^*)$. Both sign conventions lead to valid Lie–Poisson brackets. We use the plus sign convention for the rest of this section, although we will need both signs in later chapters. The Lie–Poisson bracket $\{\cdot, \cdot\}_{\mathfrak{g}}$ is an affine Poisson bracket[3] (2.1.20) on $\mathfrak{g}^*$, with $c = [\cdot, \cdot]$ and $\Omega = 0$. If $\phi : \mathfrak{g}_1 \to \mathfrak{g}_2$ is a linear map, then ϕ is a Lie algebra homomorphism if and only if its formal linear adjoint $\phi^* : \mathfrak{g}_2^* \to \mathfrak{g}_1^*$ is a Poisson map, where $\mathfrak{g}_1^*$ and $\mathfrak{g}_2^*$ are equipped with their respective Lie–Poisson brackets of the same sign ([130], Lemma 8.2).

The symmetric algebra $\mathcal{P}ol(\mathfrak{g})$ of polynomials generated by the commuting monomials $X \in \mathfrak{g}$ can be made into a Poisson algebra by extending the Lie bracket $[\cdot, \cdot]$ to polynomials through the Leibniz rule:

$$[XY, Z] := X[Y, Z] + Y[X, Z], \tag{2.2.7}$$

for all $X, Y, Z \in \mathfrak{g}$, and similarly for higher degree polynomials[4]. If one considers the polynomials in $\mathcal{P}ol(\mathfrak{g})$ as polynomial functionals on $\mathfrak{g}^*$ (for example, the monomial $XY \in$

[3]The Lie–Poisson bracket can be obtained geometrically from Poisson reduction [30, 128, 129, 130]. We discuss this example in section **2.5.1**.

[4]The symmetric algebra $\mathcal{P}ol(\mathfrak{g})$ equipped with the Lie–Poisson bracket can be considered as a "classicalisation" (being opposite to quantisation) of the universal enveloping algebra $U\mathfrak{g}$ of $\mathfrak{g}$ – $\mathcal{P}ol(\mathfrak{g})$ is the associated graded algebra of the filtered algebra $U\mathfrak{g}$. For an exposition on these algebraic objects and constructions, see [28].

$\mathscr{P}ol(\mathfrak{g})$ is mapped to the functional $m \mapsto \langle m, X\rangle\langle m, Y\rangle$), then $\mathscr{P}ol(\mathfrak{g})$ becomes a Poisson subalgebra of $\mathscr{F}(\mathfrak{g}^*)$ under the plus Lie–Poisson bracket (2.2.6).

2.2.2 Semidirect products

It is of interest in many applications to enlarge a Lie algebra $\mathfrak{g}$ in order to construct new and related Poisson brackets on a larger space. Given a Lie algebra $\mathfrak{g}$ and a representation $\phi : \mathfrak{g} \to End(V)$ on a vector space V, we can construct the *semidirect product Lie algebra* $\mathfrak{s} = \mathfrak{g} \ltimes V$. As a vector space, $\mathfrak{s}$ can be identified with $\mathfrak{g} \times V$, with typical element (X, v), where $X \in \mathfrak{g}$ and $v \in V$ The Lie bracket on $\mathfrak{s}$ is

$$[(X, v), (Y, w)] := ([X, Y], X \cdot w - Y \cdot v)\,, \tag{2.2.8}$$

for all $X, Y \in \mathfrak{g}$ and $v, w \in V$. Here we suppress the map ϕ from the notation and denote $\phi(X)w$ by $X \cdot w$ for brevity.

Let $\mathfrak{s}^*$ be the smooth dual of $\mathfrak{s}$. We can identify $\mathfrak{s}^*$ with $\mathfrak{g}^* \times V^*$ as a vector space, with typical element (m, μ), where $m \in \mathfrak{g}^*$ and $\mu \in V$. The Lie–Poisson bracket on $\mathfrak{s}^*$ is

$$\{F, G\}[m, \mu] = \left\langle m, \left[\frac{\delta F}{\delta m}, \frac{\delta G}{\delta m}\right]\right\rangle + \left\langle \mu, \frac{\delta F}{\delta m} \cdot \frac{\delta G}{\delta \mu} - \frac{\delta G}{\delta m} \cdot \frac{\delta F}{\delta \mu}\right\rangle, \tag{2.2.9}$$

where $F, G \in \mathscr{F}(\mathfrak{s}^*)$. If $\mathfrak{g}$ has multiple representation $V_1, \ldots V_a$, we can form the direct product representation by letting $X \cdot (v_1, \ldots, v_a) := (X \cdot v_1, \ldots, X \cdot v_a)$, and thus construct the semidirect product Lie algebra $\mathfrak{s} = \mathfrak{g} \ltimes (V_1 \oplus \ldots \oplus V_a)$. The smooth dual $\mathfrak{s}^*$ can be identified with $\mathfrak{g}^* \times V_1^* \times \ldots \times V_a^*$ as a vector space, with typical element $(m, \mu_1, \ldots, \mu_a)$, where $m \in \mathfrak{g}^*$ and $\mu_i \in V_i^*$. The Lie–Poisson bracket on $\mathfrak{s}^*$ is

$$\{F, G\}_{\mathfrak{s}}[m, \mu_1, \ldots, \mu_a] = \left\langle m, \left[\frac{\delta F}{\delta m}, \frac{\delta G}{\delta m}\right]\right\rangle + \sum_{i=1}^{a} \left\langle \mu_a, \frac{\delta F}{\delta m} \cdot \frac{\delta G}{\delta \mu_a} - \frac{\delta G}{\delta m} \cdot \frac{\delta F}{\delta \mu_a}\right\rangle, \tag{2.2.10}$$

where $F, G \in \mathscr{F}(\mathfrak{s}^*)$.

There is a slight generalisation to the semidirect product construction. Let $\mathfrak{h}$ be a Lie algebra. A *derivation* on $\mathfrak{h}$ is a linear map $D : \mathfrak{h} \to \mathfrak{h}$ that satisfies

$$D\left([H, K]\right) = [D(H), K] + [H, D(K)], \tag{2.2.11}$$

for all $H, K \in \mathfrak{h}$. The space of derivations on $\mathfrak{h}$ is denoted $Der(\mathfrak{h})$, and it is a Lie algebra: given $D_1, D_2 \in Der(\mathfrak{h})$, we can directly verify that $D_1D_2 - D_2D_1$ is also a derivation. The linear map $ad(H)$ for any $H \in \mathfrak{h}$ is always a derivation by the Jacobi identity (2.2.1), and such derivations are called *inner derivations*.

Now let $\phi : \mathfrak{g} \to Der(\mathfrak{h})$ be a Lie algebra homomorphism. Then $\mathfrak{h}$ is a representation of $\mathfrak{g}$, with the additional property that $X \cdot [H, K] = [X \cdot H, K] + [H, X \cdot K]$. We can define the *semidirect product Lie algebra* $\mathfrak{s} = \mathfrak{g} \ltimes \mathfrak{h}$ as the Lie algebra whose underlying vector space is $\mathfrak{g} \times \mathfrak{h}$ and has the Lie bracket

$$[(X, H), (Y, K)] := ([X, Y], X \cdot K - Y \cdot H + [H, K]) , \tag{2.2.12}$$

for all $X, Y \in \mathfrak{g}$ and $H, K \in \mathfrak{h}$. The Jacobi identity for this bracket can be verified directly – the derivation property of the action of $\mathfrak{g}$ on $\mathfrak{h}$ is crucial. If $\mathfrak{h}$ is an abelian Lie algebra, then $Der(\mathfrak{h}) = End(\mathfrak{h})$ and we recover the semidirect product Lie algebra defined in (2.2.8). The smooth dual $\mathfrak{s}^*$ can be identified with $\mathfrak{g}^* \times \mathfrak{h}^*$ as a vector space, with typical element (m, μ), where $m \in \mathfrak{g}^*$ and $\mu \in \mathfrak{h}^*$. The Lie–Poisson bracket on $\mathfrak{s}^*$ is

$$\{F, G\}_{\mathfrak{s}}[m, \mu] = \left\langle m, \left[\frac{\delta F}{\delta m}, \frac{\delta G}{\delta m}\right]\right\rangle + \left\langle \mu, \frac{\delta F}{\delta m} \cdot \frac{\delta G}{\delta \mu} - \frac{\delta G}{\delta m} \cdot \frac{\delta F}{\delta \mu} + \left[\frac{\delta F}{\delta \mu}, \frac{\delta G}{\delta \mu}\right]\right\rangle , \tag{2.2.13}$$

where $F, G \in \mathcal{F}(\mathfrak{s}^*)$.

2.2.3 Cocycles, central extensions and Lie algebra cohomology

In this section we explain the notion of a 2-cocycle on a Lie algebra, which shows up as the constant part of an affine Poisson bracket. The terminology comes from the theory of *Lie algebra cohomology*. The classical reference is [40], with [107, 114] being modern references that emphasise applications in Poisson geometry and Poisson algebras. In the following, $\mathfrak{g}$ is a fixed Lie algebra, V is a representation of $\mathfrak{g}$, and we denote the action of $X \in \mathfrak{g}$ on $v \in V$ by $X \cdot v$.

Let $C^k(\mathfrak{g}; V)$ be the space of skew-symmetric k-linear forms on $\mathfrak{g}$ with values in a representation V. We set $C^0(\mathfrak{g}; V) = V$ and $C^m(\mathfrak{g}; V) = 0$ for $m < 0$ by convention. Consider the map $\delta^k : C^k(\mathfrak{g}; V) \to C^{k+1}(\mathfrak{g}; V)$ defined as follows:

$$\begin{aligned}\delta^k \alpha(X_0, X_1, \ldots, X_k) := &\sum_{i=0}^{k} (-1)^i X_i \cdot \alpha\left(X_0, \ldots, \hat{X}_i, \ldots, X_k\right) \\ &+ \sum_{0 \le i < j \le k} (-1)^{i+j} \alpha\left([X_i, X_j], X_0, \ldots, \hat{X}_i, \ldots, \hat{X}_j, \ldots, X_k\right) ,\end{aligned} \tag{2.2.14}$$

where $\alpha \in C^k(\mathfrak{g}; V)$, and the hat indicates an omitted argument. One can check that $\delta^{k+1}\delta^k : C^k(\mathfrak{g}; V) \to C^{k+2}(\mathfrak{g}; V)$ is 0, so $C^\cdot(\mathfrak{g}; V) := \oplus_k C^k(\mathfrak{g}; V)$ is a cochain complex,

which is called the *Chevalley–Eilenberg complex of* $\mathfrak{g}$ *with coefficients in* V. As usual, define

$$Z^k(\mathfrak{g};V) := \ker \delta^k = \{\alpha \in C^k(\mathfrak{g};V) : \delta^k \alpha = 0\}, \tag{2.2.15a}$$

$$B^k(\mathfrak{g};V) := \mathrm{im}\delta^{k-1} = \{\delta^{k-1}\beta : \beta \in C^{k-1}(\mathfrak{g};V)\}, \tag{2.2.15b}$$

$$H^k(\mathfrak{g};V) := Z^k(\mathfrak{g};V)/B^k(\mathfrak{g};V) \quad . \tag{2.2.15c}$$

Elements in $Z^k(\mathfrak{g};V)$ are called k*-cocycles of* $\mathfrak{g}$ *with coefficients in* V, elements in $B^k(\mathfrak{g};V)$ are called k*-coboundaries of* $\mathfrak{g}$ *with coefficients in* V, and the space $H^k(\mathfrak{g};V)$ is called the k^{th} *cohomology group of* $\mathfrak{g}$ *with coefficients in* V. The cohomology group $H^k(\mathfrak{g};V)$ is always well-defined, because $B^k(\mathfrak{g};V)$ is always a vector subspace of $Z^k(\mathfrak{g};V)$ by $\delta^k\delta^{k-1} = 0$.

Let us focus on the case where $V = \mathbb{R}$ and where $\mathfrak{g}$ acts trivially on $V = \mathbb{R}$. In this case, the phrase "with coefficients in $\mathbb{R}$" is often omitted when the context is clear. Elements in $Z^k(\mathfrak{g};\mathbb{R})$ are then simply called k-cocycles, and similarly for the elements in $B^k(\mathfrak{g};\mathbb{R})$ and $H^k(\mathfrak{g};\mathbb{R})$.

For $k = 0$, the map δ^0 is the zero map, so $H^0(\mathfrak{g},\mathbb{R}) = Z^0(\mathfrak{g};\mathbb{R}) = C^0(\mathfrak{g},\mathbb{R}) = \mathbb{R}$ and $B^0(\mathfrak{g};\mathbb{R}) = 0$.

For $k = 1$, the map $\delta^1 : \mathfrak{g}^* \to C^2(\mathfrak{g},\mathbb{R})$ is given explicitly by

$$\delta^1 m\,(X,Y) := -m\,([X,Y])\,, \tag{2.2.16}$$

where $m \in \mathfrak{g}^*$ and $X, Y \in \mathfrak{g}$. So m is a 1-cocycle if and only if $m([X,Y]) = 0$ for all $X, Y \in \mathfrak{g}$, or more succinctly that m annihilates the commutator ideal $[\mathfrak{g},\mathfrak{g}]$ of $\mathfrak{g}$. Thus we can write $Z^1(\mathfrak{g};\mathbb{R}) = (\mathfrak{g}/[\mathfrak{g},\mathfrak{g}])^*$, and since $B^1(\mathfrak{g};\mathbb{R}) = 0$, we also have $H^1(\mathfrak{g};\mathbb{R}) = (\mathfrak{g}/[\mathfrak{g},\mathfrak{g}])^*$.

For $k = 2$, the map $\delta^2 : C^2(\mathfrak{g},\mathbb{R}) \to C^3(\mathfrak{g},\mathbb{R})$ is given explicitly by

$$\delta^2\Omega\,(X,Y,Z) := -\Omega\,([X,Y],Z) + \Omega\,([X,Z],Y) - \Omega\,([Y,Z],X)\,, \tag{2.2.17}$$

where $\Omega \in C^2(\mathfrak{g},\mathbb{R})$ and $X, Y, Z \in \mathfrak{g}$. The classical interpretation for a 2-cocycle Ω is that it defines a *central extension* $\tilde{\mathfrak{g}}$ of $\mathfrak{g}$. Let $\tilde{\mathfrak{g}}$ be the vector space $\mathfrak{g} \oplus \mathbb{R}$, and we define a skew-symmetric bilinear operation on $\tilde{\mathfrak{g}}$ by

$$[X + a, Y + b] := [X,Y] + \Omega(X,Y), \tag{2.2.18}$$

where $\Omega : \mathfrak{g} \times \mathfrak{g} \to \mathbb{R}$ is a skew-symmetric bilinear form on $\mathfrak{g}$. Then the operation defined in (2.2.18) satisfies the Jacobi identity (2.2.1) if and only if $\delta^2\Omega = 0$. An equivalent definition of a central extension can be given in terms of a short exact sequence: $\tilde{\mathfrak{g}}$ is called a *central*

extension of $\mathfrak{g}$ by $\mathbb{R}$ if there exists a short exact sequence[5] of Lie algebra homomorphisms

$$0 \to \mathbb{R} \to \tilde{\mathfrak{g}} \to \mathfrak{g} \to 0, \tag{2.2.19}$$

where $\mathbb{R}$ is considered as an abelian Lie algebra, and where the image of the first map $\mathbb{R} \to \tilde{\mathfrak{g}}$ lies in the centre $Z(\tilde{\mathfrak{g}})$. Regarding the maps in (2.2.19) as linear maps between vector spaces only, we see that $\tilde{\mathfrak{g}} = \mathfrak{g} \oplus \mathbb{R}$ as a vector space. The Lie bracket on $\tilde{\mathfrak{g}}$ can then be always written in the form (2.2.18) since the factor of $\mathbb{R}$ is in $Z(\tilde{\mathfrak{g}})$, with the additional knowledge that Ω is a 2-cocycle. Conversely, the formula (2.2.18) defines a central extension in the sense of (2.2.19) whenever Ω is a 2-cocycle.

Two central extensions $\tilde{\mathfrak{g}}_1$ and $\tilde{\mathfrak{g}}_2$ are *equivalent* if there is a commutative diagram of Lie algebra homomorphisms

$$\begin{array}{ccccccccc} 0 & \to & \mathbb{R} & \to & \tilde{\mathfrak{g}}_1 & \to & \mathfrak{g} & \to & 0 \\ & & \downarrow \mathrm{id} & & \downarrow \phi & & \downarrow \mathrm{id} & & \\ 0 & \to & \mathbb{R} & \to & \tilde{\mathfrak{g}}_2 & \to & \mathfrak{g} & \to & 0 \end{array} \tag{2.2.20}$$

where the top and bottom rows are the respective short exact sequences that define $\tilde{\mathfrak{g}}_1$ and $\tilde{\mathfrak{g}}_2$, id denotes the identity map, and $\phi : \tilde{\mathfrak{g}}_1 \to \tilde{\mathfrak{g}}_2$ is an isomorphism. Regarding both central extensions as $\mathfrak{g} \oplus \mathbb{R}$, the map ϕ must take the form $X + a \mapsto X + (a + m(X))$ by the requirements of (2.2.20), where $m \in \mathfrak{g}^*$. If Ω_1 and Ω_2 are the two 2-cocycles that define the central extensions $\tilde{\mathfrak{g}}_1$ and $\tilde{\mathfrak{g}}_2$ respectively, then requiring ϕ to be a homomorphism gives

$$\phi\left([X,Y] + \Omega_1(X,Y)\right) = [X,Y] + \Omega_1(X,Y) + m([X,Y]) = [X,Y] + \Omega_2(X,Y), \tag{2.2.21}$$

so $\Omega_2 - \Omega_1 = -\delta^1 m$ is a 2-coboundary. Conversely, if the two 2-cocycles of two central extensions $\tilde{\mathfrak{g}}_1$ and $\tilde{\mathfrak{g}}_2$ differ by a 2-coboundary, the above formula for ϕ gives an isomorphism between $\tilde{\mathfrak{g}}_1$ and $\tilde{\mathfrak{g}}_2$ that fits into the commutative diagram (2.2.20). There is therefore a one-to-one correspondence between the central extensions of $\mathfrak{g}$ by $\mathbb{R}$ up to equivalence (2.2.20) and the elements of the second cohomology group $H^2(\mathfrak{g};\mathbb{R})$ of $\mathfrak{g}$ with coefficients in $\mathbb{R}$.

As we have seen in section **2.1.3**, affine Poisson brackets are in one-to-one correspondence with Lie algebras equipped with a 2-cocycle. Let us consider two affine Poisson brackets on $\mathfrak{g}^*$ given by the Lie–Poisson bracket plus a 2-cocycle:

$$\{F,G\}_i = \left\langle m, \left[\frac{\delta F}{\delta m}, \frac{\delta G}{\delta m}\right]\right\rangle + \Omega_i\left(\frac{\delta F}{\delta m}, \frac{\delta G}{\delta m}\right), \tag{2.2.22}$$

[5]The term "short exact sequence" comes from homological algebra; in our context it means that the first map $\mathbb{R} \to \tilde{\mathfrak{g}}$ is an injective Lie algebra homomorphism, the second map $\tilde{\mathfrak{g}} \to \mathfrak{g}$ is a surjective Lie algebra homomorphism, and that the kernel of $\tilde{\mathfrak{g}} \to \mathfrak{g}$ is equal to the image of $\mathbb{R} \to \tilde{\mathfrak{g}}$.

for $i = 1, 2$, where $F, G \in \mathcal{F}(\mathfrak{g}^*)$. If $\Omega_2 - \Omega_1 = \delta^1 m_0$ for some $m_0 \in \mathfrak{g}^*$, then an affine change of coordinates $m' = m + m_0$ transforms the bracket $\{\cdot,\cdot\}_1$ into the bracket $\{\cdot,\cdot\}_2$. In particular, if Ω_2 is a 2-coboundary, the bracket $\{\cdot,\cdot\}_2$ can be transformed into the Lie–Poisson bracket (2.2.6) with an affine change of coordinates.

The Lie–Poisson bracket for a central extension $\tilde{\mathfrak{g}}$ is closely related to the affine Poisson bracket on $\mathfrak{g}$ with the same 2-cocycle Ω that defines the central extension $\tilde{\mathfrak{g}}$. A typical element of $\tilde{\mathfrak{g}}^*$ is a pair (m, c), where $m \in \mathfrak{g}^*$ and $c \in \mathbb{R}$.

$$\{F, G\}_{\tilde{\mathfrak{g}}}[m, c] = \left\langle m, \left[\frac{\delta F}{\delta m}, \frac{\delta G}{\delta m}\right]\right\rangle + c\Omega\left(\frac{\delta F}{\delta m}, \frac{\delta G}{\delta m}\right), \tag{2.2.23}$$

where $F, G \in \mathcal{F}(\tilde{\mathfrak{g}}^*)$. Any function of c only is a Casimir function of $\{\cdot,\cdot\}_{\tilde{\mathfrak{g}}}$. The level set $c = 1$ is a Poisson submanifold, and the restriction of the Poisson bracket to $c = 1$ is precisely the affine Poisson bracket on $\mathfrak{g}^*$ given by the Lie–Poisson bracket plus the 2-cocycle Ω.

2.2.4 Cocycles in semidirect products

As an application of the ideas in section **2.2.3**, consider the semidirect product Lie algebra $\mathfrak{g} \ltimes V$. Let us consider the representation V as an abelian Lie algebra, and consider a skew-symmetric bilinear from $\omega : V \times V \to \mathbb{R}$ that satisfies

$$\omega(X \cdot v, w) + \omega(v, X \cdot w) = 0, \tag{2.2.24}$$

for all $v, w \in V$ and all $X \in \mathfrak{g}$. Since V is abelian, any skew-symmetric bilinear form defines a central extension of V, so let $\tilde{V}$ be the central extension of V by ω. Property (2.2.24) implies that the homomorphism $\mathfrak{g} \to End(V)$ can be lifted to a homomorphism $\mathfrak{g} \to Der(\tilde{V})$, where the $\mathfrak{g}$-action is

$$X \cdot (v, a) := (X \cdot v, 0), \tag{2.2.25}$$

for all $(v, a) \in \tilde{V}$ and $X \in \mathfrak{g}$. We can therefore form the semidirect product Lie algebra $\mathfrak{g} \ltimes \tilde{V}$. Its smooth dual space can be taken as $(\mathfrak{g} \ltimes \tilde{V})^* = \mathfrak{g}^* \times V^* \times \mathbb{R}$, with typical element (m, μ, c) where $m \in \mathfrak{g}^*$, $\mu \in V$ and $c \in \mathbb{R}$. The Lie–Poisson bracket on $(\mathfrak{g} \ltimes \tilde{V})^*$ is

$$\begin{aligned}&\{F, G\}_{\mathfrak{g}\ltimes\tilde{V}}[m, \mu, c] \\ &= \left\langle m, \left[\frac{\delta F}{\delta m}, \frac{\delta G}{\delta m}\right]\right\rangle + \left\langle \mu, \frac{\delta F}{\delta m} \cdot \frac{\delta G}{\delta \mu} - \frac{\delta G}{\delta m} \cdot \frac{\delta F}{\delta \mu}\right\rangle + c\omega\left(\frac{\delta F}{\delta \mu}, \frac{\delta G}{\delta \mu}\right),\end{aligned} \tag{2.2.26}$$

where $F, G \in \mathcal{F}((\mathfrak{g} \ltimes \tilde{V})^*)$. Any function of c only is a Casimir function of $\{\cdot,\cdot\}_{\mathfrak{g}\ltimes\tilde{V}}$. The level set $c = 1$ is therefore a Poisson submanifold. One can also check that the skew-symmetric bilinear form $\Omega : \mathfrak{g} \ltimes V \times \mathfrak{g} \ltimes V \to \mathbb{R}$, defined as the extension of ω by zero

to $\mathfrak{g} \ltimes V$, is a 2-cocycle of the semidirect product Lie algebra $\mathfrak{g} \ltimes V$. The affine Poisson bracket on $(\mathfrak{g} \ltimes V)^*$ given by the Lie–Poisson bracket plus the 2-cocycle Ω then coincides with the bracket (2.2.26) at $c = 1$.

An important case in which we have the from ω satisfying (2.2.24) is when $V = W \times W^*$ is the direct sum representation of a representation W and its dual. The Lie–Poisson bracket on $(\mathfrak{g} \ltimes (W \times W^*))^*$ plus the 2-cocycle ω is is

$$\begin{aligned}\{F, G\}[m, \alpha, w] = &\left\langle m, \left[\frac{\delta F}{\delta m}, \frac{\delta G}{\delta m}\right]\right\rangle + \left\langle \alpha, \frac{\delta F}{\delta m} \cdot \frac{\delta G}{\delta \alpha} - \frac{\delta G}{\delta m} \cdot \frac{\delta F}{\delta \alpha}\right\rangle \\ &+ \left\langle w, \frac{\delta F}{\delta m} \cdot \frac{\delta G}{\delta w} - \frac{\delta G}{\delta m} \cdot \frac{\delta F}{\delta w}\right\rangle + \left\langle \frac{\delta F}{\delta w}, \frac{\delta G}{\delta \alpha}\right\rangle - \left\langle \frac{\delta G}{\delta w}, \frac{\delta F}{\delta \alpha}\right\rangle,\end{aligned} \tag{2.2.27}$$

where (m, α, w) is a typical element of $(\mathfrak{g} \ltimes (W \times W^*))^* = \mathfrak{g}^* \times W^* \times W$, and $F, G \in \mathcal{F}(\mathfrak{g} \ltimes (W \times W^*))^*$. Now consider the map $\phi^* : W^* \times W \to \mathfrak{g}^*$ defined by the following formula:

$$\langle \phi^*(\alpha, w), X\rangle := \langle \alpha, X \cdot w\rangle = -\langle X \cdot \alpha, w\rangle, \tag{2.2.28}$$

for all $w \in W$, all $\alpha \in W^*$ and all $X \in \mathfrak{g}$. This map is sometimes called the diamond operator [69]. The map ϕ can be thought of as the formal linear adjoint of the map $\phi : \mathfrak{g} \to End(W)$ that defines the representation on W. Consider the following (invertible) change of variables from (m, α, w) to (m', α', w'), defined by

$$m = m' + \phi^*(\alpha', w'), \quad \alpha = \alpha', \quad w = w', \tag{2.2.29}$$

then for a functional $F[m, \alpha, w] = F[m', \alpha', w']$, its functional derivatives transform as

$$\frac{\delta F}{\delta m'} = \frac{\delta F}{\delta m}, \quad \frac{\delta F}{\delta \alpha'} = \frac{\delta F}{\delta \alpha} + \frac{\delta F}{\delta m} \cdot w', \quad \frac{\delta F}{\delta w'} = \frac{\delta F}{\delta w} - \frac{\delta F}{\delta m} \cdot \alpha', \tag{2.2.30}$$

by the functional chain rule. A straightforward computation then shows that the affine Poisson bracket (2.2.27) transforms into the following particularly simple form:

$$\{F, G\}[m', \alpha', w'] = \left\langle m', \left[\frac{\delta F}{\delta m'}, \frac{\delta G}{\delta m'}\right]\right\rangle + \left\langle \frac{\delta F}{\delta w'}, \frac{\delta G}{\delta \alpha'}\right\rangle - \left\langle \frac{\delta G}{\delta w'}, \frac{\delta F}{\delta \alpha'}\right\rangle, \tag{2.2.31}$$

where $F, G \in \mathcal{F}(\mathfrak{g}^* \times W^* \times W)$. We can also interpret this result as saying that ω is a 2-cocycle on the direct product Lie algebra $\mathfrak{g} \times W \times W^*$, where W and W^* are considered as abelian Lie algebras.

2.2.5 Formal series, path algebras and loop algebras

In this section we study two constructions that enlarge a Lie algebra with a formal parameter. Each construction has a differential-geometric relative that can be defined as the space of maps from a one-dimensional space into the Lie algebra. In the following, $\mathfrak{g}$ is a fixed Lie algebra.

Consider the space $\mathfrak{g}[[\epsilon]]$ of formal power series with coefficients in $\mathfrak{g}$. A typical element in $\mathfrak{g}[[\epsilon]]$ is a formal power series $\sum_{a=0}^{\infty} X_a \epsilon^a$, where $X_a \in \mathfrak{g}$. The Lie bracket on $\mathfrak{g}[[\epsilon]]$ is

$$\left[\sum_{a=0}^{\infty} X_a \epsilon^a, \sum_{b=0}^{\infty} Y_b \epsilon^b\right] := \sum_{c=0}^{\infty} \sum_{\substack{a+b=c \\ a\geq 0, b\geq 0}} [X_a, Y_b]\, \epsilon^c, \tag{2.2.32}$$

where $X_a, Y_b \in \mathfrak{g}$. For $k \geq 0$, consider the Lie ideal

$$\langle \epsilon^{k+1} \rangle := \left\{ \sum_{a=0}^{\infty} X_a \epsilon^a : X_0 = \ldots = X_k = 0. \right\} \tag{2.2.33}$$

The resulting quotient Lie algebra $\mathfrak{g}[[\epsilon]]/\langle \epsilon^{k+1} \rangle$ is the Lie algebra of formal power series modulo ϵ^{k+1} with coefficients in $\mathfrak{g}$. A typical element of $\mathfrak{g}[[\epsilon]]/\langle \epsilon^{k+1} \rangle$ is a finite sum $\sum_{a=0}^{k} X_a \epsilon^a$, where $X_a \in \mathfrak{g}$. The Lie bracket on $\mathfrak{g}[[\epsilon]]/\langle \epsilon^{k+1} \rangle$ is

$$\left[\sum_{a=0}^{k} X_a \epsilon^a, \sum_{b=0}^{k} Y_b \epsilon^b\right] := \sum_{c=0}^{k} \sum_{\substack{a+b=c \\ a\geq 0, b\geq 0}} [X_a, Y_b]\, \epsilon^c. \tag{2.2.34}$$

In particular, $\mathfrak{g}[[\epsilon]]/\langle \epsilon^2 \rangle$ is the semidirect product Lie algebra $\mathfrak{g} \ltimes \mathfrak{g}_{ab}$, where $\mathfrak{g}_{ab}$ is the underlying vector space of $\mathfrak{g}$ endowed with the trivial Lie bracket, and $\mathfrak{g}$ acts on $\mathfrak{g}_{ab}$ by the adjoint representation.

There is a sequence of surjective Lie algebra homomorphisms

$$\mathfrak{g} = \mathfrak{g}[[\epsilon]]/\langle \epsilon^1 \rangle \leftarrow \mathfrak{g}[[\epsilon]]/\langle \epsilon^2 \rangle \leftarrow \mathfrak{g}[[\epsilon]]/\langle \epsilon^3 \rangle \leftarrow \ldots \leftarrow \mathfrak{g}[[\epsilon]], \tag{2.2.35}$$

where the map $\mathfrak{g}[[\epsilon]]/\langle \epsilon^{k+1} \rangle \to \mathfrak{g}[[\epsilon]]/\langle \epsilon^k \rangle$ is

$$X_0 + \ldots + X_{k-1}\epsilon^{k-1} + X_k \epsilon^k \mapsto X_0 + \ldots + X_{k-1}\epsilon^{k-1}, \tag{2.2.36}$$

or more succinctly taking equivalence modulo ϵ^k.

The smooth dual to $\mathfrak{g}[[\epsilon]]$ is the vector space $\mathfrak{g}^*[\eta]$ of polynomials with coefficients in $\mathfrak{g}^*$, with finite sums $\sum_{a=0}^{\infty} m_a \eta^a, m_a \in \mathfrak{g}^*$ as typical elements. The dual pairing is

$$\left\langle \sum_{a=0}^{\infty} m_a \eta^a, \sum_{a=0}^{\infty} X_a \epsilon^a \right\rangle := \sum_{a=0}^{\infty} \langle m_a, X_a \rangle, \tag{2.2.37}$$

where $m_a \in \mathfrak{g}^*$ and $X_a \in \mathfrak{g}$. The convergence of the sum is never an issue because only finitely many m_a are non-zero. The Lie–Poisson bracket on $\mathfrak{g}^*[\eta]$ is

$$\{F, G\}_{\mathfrak{g}[[\epsilon]]} = \pm \sum_{c=0}^{\infty} \left\langle m_c, \sum_{\substack{a+b=c \\ a\geq 0, b\geq 0}} \left[\frac{\delta F}{\delta m_a}, \frac{\delta G}{\delta m_b}\right] \right\rangle, \tag{2.2.38}$$

where $F, G \in \mathcal{F}(\mathfrak{g}^*[\eta])$. The right-hand side of (2.2.38) is a finite sum, because $m_c = 0$ for all sufficiently large c, so $\{F, G\}_{\mathfrak{g}[[\epsilon]]}$ is well-defined and belongs to $\mathcal{F}(\mathfrak{g}^*[\eta])$. Similarly, the smooth dual space to $\mathfrak{g}[[\epsilon]]/\langle \epsilon^{k+1} \rangle$ is the vector space $\mathfrak{g}^*[\eta]/\langle \eta^{k+1} \rangle$ of polynomials with coefficients in $\mathfrak{g}^*$ of degree at most k, with typical element $\sum_{a=0}^{\infty} m_a \eta^a, m_a \in \mathfrak{g}^*$. The dual pairing is

$$\left\langle \sum_{a=0}^{k} m_a \eta^a, \sum_{a=0}^{k} X_a \epsilon^a \right\rangle := \sum_{a=0}^{k} \langle m_a, X_a \rangle, \tag{2.2.39}$$

where $m_a \in \mathfrak{g}^*$ and $X_a \in \mathfrak{g}$. The Lie–Poisson bracket on $\mathfrak{g}^*[\eta]/\langle \eta^{k+1} \rangle$ is

$$\{F, G\}_{\mathfrak{g}[[\epsilon]]/\langle \epsilon^{k+1} \rangle} = \pm \sum_{c=0}^{k} \left\langle m_c, \sum_{\substack{a+b=c \\ a\geq 0, b\geq 0}} \left[\frac{\delta F}{\delta m_a}, \frac{\delta G}{\delta m_b}\right] \right\rangle, \tag{2.2.40}$$

where $F, G \in \mathcal{F}(\mathfrak{g}^*[\eta]/\langle \eta^{k+1} \rangle)$. Dualising the sequence (2.2.35) gives the sequence of injective Poisson maps

$$\mathfrak{g}^* = \mathfrak{g}^*[\eta]/\langle \eta^1 \rangle \hookrightarrow \mathfrak{g}^*[\eta]/\langle \eta^2 \rangle \hookrightarrow \mathfrak{g}[\eta]/\langle \eta^3 \rangle \hookrightarrow \ldots \hookrightarrow \mathfrak{g}^*[\eta], \tag{2.2.41}$$

where the inclusion $\mathfrak{g}^*[[\eta]]/\langle \eta^k \rangle \hookrightarrow \mathfrak{g}^*[[\eta]]/\langle \eta^{k+1} \rangle$ is just the inclusion of polynomials of degree at most $k-1$ into the space of polynomials of degree at most k.

The differential-geometric relative to $\mathfrak{g}[[\epsilon]]$ is the *path algebra* $P\mathfrak{g}$, which is the space of sufficiently regular maps from a fixed (small) interval $I \in \mathbb{R}$ containing 0 to $\mathfrak{g}$, often endowed with a suitable topology when $\mathfrak{g}$ is a Banach space or a Fréchet space. The Lie bracket on $P\mathfrak{g}$ is defined pointwise: if $X(\epsilon)$ and $Y(\epsilon)$ are $\mathfrak{g}$-valued paths, their Lie bracket is the $\mathfrak{g}$-valued path $[X(\epsilon), Y(\epsilon)]$. If we expand $X(\epsilon)$ and $Y(\epsilon)$ as a power series in ϵ, we would obtain the Lie bracket (2.2.32) for the coefficients of the expansion $X(\epsilon) = X_0 + X_1\epsilon + X_2\epsilon^2 + \ldots$. The power series obtained this way would be convergent in a suitable sense, so we cannot identify $\mathfrak{g}[[\epsilon]]$ with $P\mathfrak{g}$ exactly.

A different but equally interesting construction is the space $\mathfrak{g}[z, z^{-1}]$ of *Laurent polynomials* with coefficients in $\mathfrak{g}$. The elements of $\mathfrak{g}[z, z^{-1}]$ are formal sums $\sum_{a=-\infty}^{\infty} X_a z^a$, where $X_a \in \mathfrak{g}$ and all but finitely many X_a are zero. The Lie bracket is

$$\left[\sum_{a=-\infty}^{\infty} X_a z^a, \sum_{b=-\infty}^{\infty} Y_b z^b\right] := \sum_{c=-\infty}^{\infty} \sum_{a+b=c} [X_a, Y_b]\, z^c, \tag{2.2.42}$$

where $X_a, Y_b \in \mathfrak{g}[z, z^{-1}]$. Consider also the space $\mathfrak{g}((z))$ of *formal Laurent series* with coefficients in $\mathfrak{g}$, which is the space of all formal sums $\sum_{a=-\infty}^{\infty} X_a z^a$, where $X_a \in \mathfrak{g}$ and all but finitely many X_a for $a < 0$ are zero. The formula (2.2.42) also defines a Lie bracket on $\mathfrak{g}((z))$, because the coefficient for any z^c is always a finite sum. We cannot define a Lie bracket on the space of Laurent series that extend infinitely on both sides in a purely algebraic manner however, since the coefficients for z^c would then involve infinite sums in $\mathfrak{g}$, which does not make sense in the absence of analytical structures on $\mathfrak{g}$.

The Lie algebra of formal power series $\mathfrak{g}[[z]]$ is a subalgebra of $\mathfrak{g}((z))$. In fact, $\mathfrak{g}((z))$ can be decomposed into a direct sum of subalgebras $\mathfrak{g}((z)) = \mathfrak{g}[[z]] \oplus z^{-1}\mathfrak{g}[z^{-1}]$, where $z^{-1}\mathfrak{g}[z^{-1}]$ is the subalgebra of formal Laurent series whose coefficients X_a are only non-zero for negative a.

The differential-geometric relative to $\mathfrak{g}[z, z^{-1}]$ is the *loop algebra* $L\mathfrak{g}$, which consists of sufficiently regular maps from the unit circle S^1 to $\mathfrak{g}$. If $\mathfrak{g}$ is a Banach space or a Fréchet space, the loop algebra $L\mathfrak{g}$ is often endowed with a suitable topology. The Lie bracket on $L\mathfrak{g}$ is defined pointwise: if $X(\theta)$ and $Y(\theta)$ are $\mathfrak{g}$-valued loops, their Lie bracket is the $\mathfrak{g}$-valued loop $[X(\theta), Y(\theta)]$. By expanding $X(\theta)$ and $Y(\theta)$ in a Fourier series[6] $X(\theta) = \sum_{a=-\infty}^{\infty} X_a \mathrm{e}^{\mathrm{i}a\theta}, Y(\theta) = \sum_{a=-\infty}^{\infty} Y_b \mathrm{e}^{\mathrm{i}b\theta}$, we recover the Lie bracket (2.2.42) with the substitution $z = \mathrm{e}^{\mathrm{i}\theta}$. The main difference between $L\mathfrak{g}$ and $\mathfrak{g}((z))$ is that the Fourier series in $L\mathfrak{g}$ extend to both sides but converge in an appropriate sense, whereas the formal Laurent series in $\mathfrak{g}((z))$ extend to the positive side only. A Laurent polynomial in $\mathfrak{g}[z, z^{-1}]$ can be included into the complexification of $L\mathfrak{g}$ as a finite Fourier series.

The smooth dual of $L\mathfrak{g}$ can be taken as $L\mathfrak{g}^*$, the space of $\mathfrak{g}$-valued loops $m : S^1 \to \mathfrak{g}^*$, with the dual pairing given by integrating the pointwise dual pairing:

$$\langle m, X \rangle = \int_0^{2\pi} d\theta \, \langle m(\theta), X(\theta) \rangle, \tag{2.2.43}$$

where $m = m(\theta) \in L\mathfrak{g}^*$ and $X = X(\theta) \in L\mathfrak{g}$. The Lie–Poisson bracket on $L\mathfrak{g}^*$ is

$$\{F, G\}_{L\mathfrak{g}} = \int_0^{2\pi} d\theta \, \left\langle m(\theta), \left[\frac{\delta F}{\delta m}(\theta), \frac{\delta G}{\delta m}(\theta) \right] \right\rangle, \tag{2.2.44}$$

where $F, G \in \mathcal{F}(L\mathfrak{g}^*)$.

There is a dual pairing for $\mathfrak{g}((z))$ and its smooth dual that is the formal equivalent of integration on S^1. Consider the space $\mathfrak{g}^*((z))$ of formal Laurent series with coefficients in $\mathfrak{g}^*$. The dual pairing between $\mathfrak{g}$ and $\mathfrak{g}^*$ extends to a bilinear pairing $T : \mathfrak{g}((z)) \times \mathfrak{g}^*((z)) \to$

[6]The coefficients of the Fourier series X_a, Y_b are in the complexification of $\mathfrak{g}$.

$\mathbb{R}((z))$, where $\mathbb{R}((z))$ is the space of formal Laurent series with real coefficients. The explicit formula is

$$T\left(\sum_{a=-\infty}^{\infty} m_a z^a, \sum_{b=-\infty}^{\infty} X_b z^b\right) := \sum_{c=-\infty}^{\infty} \sum_{a+b=c} \langle m_a, X_b \rangle \, z^c, \tag{2.2.45}$$

where $m_a \in \mathfrak{g}^*$ and $X_b \in \mathfrak{g}$. The right-hand side of (2.2.45) is a well-defined formal Laurent series with real coefficients, since each coefficient of z^c is a finite sum, and the coefficients are all zero for sufficiently large and negative c. Define the *formal residue* $\mathrm{res} : \mathbb{R}((z)) \to \mathbb{R}$ to be the coefficient of the z^{-1} term of the formal Laurent series:

$$\mathrm{res}\left(\sum_{a=-\infty}^{\infty} f_a z^a\right) = f_{-1}, \tag{2.2.46}$$

where $\sum_{a=-\infty}^{\infty} f_a z^a \in \mathbb{R}((z))$. The formal residue can also be more abstractly defined as the cokernel of the derivation $\partial/\partial z : \mathbb{R}((z)) \to \mathbb{R}((z))$. We define a weakly non-degenerate bilinear pairing between $\mathfrak{g}((z))$ and $\mathfrak{g}^*((z))$ in terms of T and res:

$$\begin{aligned}\left\langle \sum_{a=-\infty}^{\infty} m_a z^a, \sum_{b=-\infty}^{\infty} X_b z^b \right\rangle &:= \mathrm{res}\left(z^{-1} T\left(\sum_{a=-\infty}^{\infty} m_a z^a, \sum_{b=-\infty}^{\infty} X_b z^b\right)\right) \\ &= \sum_{b=-\infty}^{\infty} \langle m_b, X_{-b} \rangle \, .\end{aligned} \tag{2.2.47}$$

The analogy between (2.2.47) and (2.2.44) is explained by complex analysis: Let $f : U \subset \mathbb{C} \to \mathbb{C}$ be a function of a complex variable that is holomorphic on the punctured unit disc on $\mathbb{C}$. Then

$$\int_0^{2\pi} d\theta \; f\left(\mathrm{e}^{\mathrm{i}\theta}\right) = \oint_{S^1} \frac{dz}{\mathrm{i}z} \, f(z) = 2\pi \mathrm{res}\left(z^{-1} f(z), z = 0\right). \tag{2.2.48}$$

Care must be taken in choosing the space of suitable functionals $\mathcal{F}[\mathfrak{g}^*((z))]$. The functional derivative of $F \in \mathcal{F}[\mathfrak{g}^*((z))]$ should take values in the smooth dual $\mathfrak{g}((z))$ of $\mathfrak{g}^*((z))$. If we write $F[m] = F[\ldots, m_{-1}, m_0, m_1, \ldots]$, then its functional derivative is the series

$$\frac{\delta F}{\delta m} = \sum_{a=-\infty}^{\infty} \frac{\delta F}{\delta m_{-a}} z^a, \tag{2.2.49}$$

which is a $\mathfrak{g}$-valued formal Laurent series if and only if $\delta F / \delta m_a = 0$ for all sufficiently large positive a. The Lie–Poisson bracket for two suitable functionals $F, G \in \mathcal{F}[\mathfrak{g}^*((z))]$ is then

$$\{F, G\}_{\mathfrak{g}((z))} = \pm \sum_{c=-\infty}^{\infty} \left\langle m_c, \sum_{a+b=c} \left[\frac{\delta F}{\delta m_a}, \frac{\delta G}{\delta m_b}\right] \right\rangle. \tag{2.2.50}$$

One can check that $\delta\{F,G\}_{\mathfrak{g}((z))}/\delta m_c = 0$ for sufficiently large positive c if $\delta F/\delta m_a$ and $\delta G/\delta m_a$ both vanish for sufficiently large positive a, so the space of suitable functionals $\mathcal{F}[\mathfrak{g}^*((z))]$ is a Poisson algebra.

2.2.6 Invariant symmetric bilinear forms

A symmetric bilinear form $B : \mathfrak{g} \times \mathfrak{g} \to \mathbb{R}$ on a Lie algebra $\mathfrak{g}$ is called *invariant* if the following identity holds:

$$B([X,Y],Z) = B(X,[Y,Z]), \tag{2.2.51}$$

for all $X, Y, Z \in \mathfrak{g}$. Such a symmetric bilinear form defines a skew-symmetric trilinear form $T_B : \mathfrak{g} \times \mathfrak{g} \times \mathfrak{g} \to \mathbb{R}$, given by

$$T_B(X,Y,Z) := B([X,Y],Z), \tag{2.2.52}$$

for all $X, Y, Z \in \mathfrak{g}$. T_B is a 3-cocycle with coefficients in $\mathbb{R}$ for the Lie algebra $\mathfrak{g}$, as the identity $\delta^3 T_B = 0$ can be directly verified (see section **2.2.3**). A Lie algebra with a weakly non-degenerate symmetric invariant bilinear form B is called a *quadratic Lie algebra*. Given a quadratic Lie algebra $\mathfrak{g}$, we can choose its smooth dual to be $\mathfrak{g}$ itself, with the dual pairing given by its weakly non-degenerate symmetric invariant bilinear form B. We can thus endow $\mathfrak{g}$ with the Lie–Poisson bracket

$$\{F,G\}_{\mathfrak{g}}[X] = B\left(X, \left[\frac{\delta F}{\delta X}, \frac{\delta G}{\delta X}\right]\right) = B\left(\left[\frac{\delta F}{\delta X}, X\right], \frac{\delta G}{\delta X}\right), \tag{2.2.53}$$

where $F, G \in \mathcal{F}(\mathfrak{g})$. Here $\delta F/\delta X$ and $\delta G/\delta X$ take values in $\mathfrak{g}$ and are defined by

$$B\left(\frac{\delta F}{\delta X}, Y\right) = \lim_{\epsilon \to 0} \frac{F[X+\epsilon Y] - F[X]}{\epsilon}, \tag{2.2.54}$$

for $X, Y \in \mathfrak{g}$. Now consider the functional $C_B[X] = B(X,X)/2$. The Lie–Poisson bracket (2.2.53) can also be written in term of T_B (2.2.52) as

$$\{F,G\}_{\mathfrak{g}}[X] = T_B\left(\frac{\delta C_B}{\delta X}, \frac{\delta F}{\delta X}, \frac{\delta G}{\delta X}\right), \tag{2.2.55}$$

so $C_B[X]$ is always a Casimir functional by the skew-symmetry of T_B.

There are many examples for quadratic Lie algebras in finite dimensions: the compact real form of any semisimple complex Lie algebra is a quadratic Lie algebra under the Killing form, and the abelian Lie algebra $\mathbb{R}^n$ is quadratic under any symmetric non-degenerate bilinear form e.g. the Euclidean inner product. The semidirect product $\mathfrak{g} \ltimes \mathfrak{g}^*$ is another example of a quadratic Lie algebra, where $\mathfrak{g}$ acts on its smooth dual $\mathfrak{g}^*$ by the coadjoint

representation. There is a weakly non-degenerate invariant symmetric bilinear form on $\mathfrak{g} \ltimes \mathfrak{g}^*$, called the *polarisation form*

$$P\left((X,m),(Y,n)\right) := \langle m, Y\rangle + \langle n, X\rangle\,, \tag{2.2.56}$$

where $X, Y \in \mathfrak{g}$ and $m, n \in \mathfrak{g}^*$.

Given an invariant symmetric bilinear form B on a Lie algebra $\mathfrak{g}$, we can extend B naturally to the Lie algebra $\mathfrak{g}[[\epsilon]]$ of formal power series, where it becomes as a $\mathbb{R}[[\epsilon]]$-valued bilinear form (also denoted B):

$$B\left(\sum_{a=0}^{\infty} X_a\epsilon^a, \sum_{b=0}^{\infty} Y_b\epsilon^b\right) := \sum_{c=0}^{\infty} \sum_{\substack{a+b=c\\ a\geq 0, b\geq 0}} B\left(X_a, Y_b\right)\epsilon^c, \tag{2.2.57}$$

where $X_a, Y_b \in \mathfrak{g}$. The extended bilinear form B is invariant in the sense that equation (2.2.51) is satisfied on the ring $\mathbb{R}[[\epsilon]]$. A similar construction defines a $\mathbb{R}[[\epsilon]]/\langle\epsilon^{k+1}\rangle$-valued invariant symmetric bilinear form B on $\mathfrak{g}[[\epsilon]]/\langle\epsilon^{k+1}\rangle$. Each coefficient of ϵ^c for B defines an invariant symmetric bilinear form on $\mathfrak{g}[[\epsilon]]$, which we denote by $B_c : \mathfrak{g}[[\epsilon]] \times \mathfrak{g}[[\epsilon]] \to \mathbb{R}$:

$$B_c\left(\sum_{a=0}^{\infty} X_a\epsilon^a, \sum_{b=0}^{\infty} Y_b\epsilon^b\right) := \sum_{\substack{a+b=c\\ a\geq 0, b\geq 0}} B\left(X_a, Y_b\right), \tag{2.2.58}$$

where $X_a, Y_b \in \mathfrak{g}$. Similarly, we can define the invariant symmetric bilinear forms $B_0, \ldots, B_k$ in $\mathfrak{g}[[\epsilon]]/\langle\epsilon^{k+1}\rangle$ with the same formula (2.2.58). If B is weakly non-degenerate on $\mathfrak{g}$, then B_k is weakly non-degenerate on $\mathfrak{g}[[\epsilon]]/\langle\epsilon^{k+1}\rangle$, but $B_0, \ldots B_{k-1}$ all have non-zero kernel.

We can also extend B to an invariant symmetric bilinear form on the loop algebra $L\mathfrak{g}$ (also denoted B), given by

$$B(X,Y) := \int_0^{2\pi} d\theta\; B(X(\theta), Y(\theta)), \tag{2.2.59}$$

where $X, Y : S^1 \to \mathfrak{g}$ are $\mathfrak{g}$-valued loops. More interestingly, any invariant symmetric bilinear form B on $\mathfrak{g}$ induces a 2-cocycle $\Omega_B : L\mathfrak{g} \times L\mathfrak{g} \to \mathrm{R}$ on $L\mathfrak{g}$, defined by the formula

$$\Omega_B(X,Y) = \int_0^{2\pi} d\theta\; B\left(X(\theta), \frac{\partial}{\partial\theta}Y(\theta)\right), \tag{2.2.60}$$

where $X, Y : S^1 \to \mathfrak{g}$ are $\mathfrak{g}$-valued loops. One can check that Ω_B is a 2-cocycle using the identity (2.2.51) and integrating by parts. The analogue of the 2-cocycle (2.2.60) on the Lie algebra $\mathfrak{g}((z))$ of formal Laurent series is

$$\Omega_B^{((z))}(X,Y) = \mathrm{res}\left(B\left(X(z), \frac{\partial}{\partial z}Y(z)\right)\right), \tag{2.2.61}$$

where $X, Y \in \mathfrak{g}((z))$ are $\mathfrak{g}$-valued formal Laurent series, B is extended to $\mathfrak{g}((z))$ as a $\mathbb{R}((z))$-valued bilinear form in the obvious way, and $\partial/\partial z$ is the obvious extension of $\partial/\partial z : \mathbb{R}((z)) \to \mathbb{R}((z))$ to $\mathfrak{g}((z))$.

2.3 Infinite-dimensional Lie algebras in differential geometry

Differential geometry is full of examples of infinite-dimensional Lie algebras. Many of them are spaces of sections of some vector bundle over a finite-dimensional manifold. The smooth dual spaces of these Lie algebras, equipped with the Lie–Poisson bracket, occurs frequently in the Hamiltonian description of fluid dynamics and kinetic theory. The main references for this section are [94, 127, 128, 129, 130]. We will assume basic familiarity with the theory of smooth manifolds. In the following, M is an orientable smooth manifold with finite dimension n.

2.3.1 The Lie algebra $\mathrm{Vect}(M)$

The most important infinite-dimensional Lie algebra associated with a manifold M is the *Lie algebra of vector fields* $\mathrm{Vect}(M)$. Let u be a vector field. In a neighbourhood U with local coordinates $x^1, \dots, x^n$, u is a first-order differential operator of the form

$$u = u^i(x) \frac{\partial}{\partial x^i}, \tag{2.3.1}$$

where $u^i(x)$ are functions on U. The Lie bracket $[u, v]$ of two vector fields u, v is defined as the commutator of u and v as first-order differential operators. It is easily checked that $[u, v]$ is also a first-order differential operator, whose local expression on U is

$$[u, v] = \left(u^j \frac{\partial v^i}{\partial x^j} - v^j \frac{\partial u^i}{\partial x^j} \right) \frac{\partial}{\partial x^i}. \tag{2.3.2}$$

The operation $[\cdot, \cdot] : \mathrm{Vect}(M) \times \mathrm{Vect}(M) \to \mathrm{Vect}(M)$ is manifestly bilinear and skew-symmetric. We can also check that $[\cdot, \cdot]$ satisfies the Jacobi identity (2.2.1), so it defines a Lie bracket.

2.3.2 The Lie derivative on tensors

Let TM and T^*M denote the tangent and cotangent bundles of M, respectively. Consider the tensor bundle $(\otimes^a TM) \otimes (\otimes^b T^*M)$. A section $A \in \Gamma((\otimes^a TM) \otimes (\otimes^b T^*M))$ is called a *tensor of rank* (a, b). Such a section corresponds to a tensor $A^{i_1 \dots i_a}_{j_1 \dots j_b}(x)$ in classical tensor

calculus. Indeed, in a coordinate neighbourhood U with local coordinates $x^1, \ldots, x^n$, the local expression for A is

$$A = A^{i_1 \ldots i_a}_{j_1 \ldots j_b}(x) \frac{\partial}{\partial x^{i_1}} \otimes \ldots \otimes \frac{\partial}{\partial x^{i_a}} \otimes dx^{j_1} \otimes \ldots \otimes dx^{j_b}, \tag{2.3.3}$$

where $A^{i_1 \ldots i_a}_{j_1 \ldots j_b}(x)$ are functions on U.

Now let u be a vector field on M. We define the *Lie derivative of the tensor A along u* to be the tensor $\mathcal{L}_u A$, given in local coordinates as

$$(\mathcal{L}_u A)^{i_1 \ldots i_a}_{j_1 \ldots j_b} = u^k \frac{\partial A^{i_1 \ldots i_a}_{j_1 \ldots j_b}}{\partial x^k} - \sum_{s=1}^{a} A^{i_1 \ldots i_{s-1} k i_{s+1} \ldots i_a}_{j_1 \ldots j_b} \frac{\partial u^{i_s}}{\partial x^k} + \sum_{s=1}^{b} A^{i_1 \ldots i_a}_{j_1 \ldots j_{s-1} k j_{s+1} \ldots j_b} \frac{\partial u^k}{\partial x^{i_s}}. \tag{2.3.4}$$

In particular, the Lie derivative of a vector field v along u is the commutator $\mathcal{L}_u v = [u, v]$. The formula (2.3.4) now defines a tensor on any coordinate neighbourhood on M. One can check that, given another coordinate neighbourhood V with coordinates $\tilde{x}^1, \ldots, \tilde{x}^n$, the expression for $\mathcal{L}_u A$ (2.3.4) transforms appropriately under a coordinate transformation $x^i \to \tilde{x}^i$ on $U \cap V$. Now cover M with coordinate neighbourhoods. The transformation property of $\mathcal{L}_u A$ on the overlaps between any two coordinate neighbourhood show that it is a tensor on all of M. Thus we have defined a map $\mathcal{L}_u : \Gamma((\otimes^a TM) \otimes (\otimes^b T^*M)) \to \Gamma((\otimes^a TM) \otimes (\otimes^b T^*M))$ that takes a tensor A to $\mathcal{L}_u A$.

The map taking a vector field u to the operator $\mathcal{L}_u$ satisfies an important identity

$$\mathcal{L}_{[u,v]} A = \mathcal{L}_u \mathcal{L}_v A - \mathcal{L}_v \mathcal{L}_u A, \tag{2.3.5}$$

where u, v are any two vector fields and A is any tensor. The space of tensors $\Gamma((\otimes^a TM) \otimes (\otimes^b T^*M))$ is therefore a representation of the Lie algebra $\mathrm{Vect}(M)$, where vector fields act on tensors by the Lie derivative. The operation $A \to \mathcal{L}_u A$ also preserves any permutation-type symmetries on the indices of A. For example, if A_{ijk} is a rank-$(0,3)$ skew-symmetric tensor (i.e. a 3-form), then so is $(\mathcal{L}_u A)_{ijk}$. The vector subspace of tensors with a given permutation-type symmetry therefore defines a subrepresentation of $\mathrm{Vect}(M)$. We can thus form semidirect product Lie algebras of the form $\mathrm{Vect}(M) \ltimes \Gamma(E)$, where E is a direct sum bundle of tensor bundles, each summand possibly having a fixed permutation-type symmetry.

Let us digress and explain the geometric interpretation of the Lie derivative briefly. Let u be a vector field. An *integral curve* of u is a curve $x^i(t)$ that satisfies the ordinary differential equation $dx^i(t)/dt = u^i(x(t))$. We claim that the formula (2.3.4) for the Lie derivative $\mathcal{L}_u A$ of a tensor A can be interpreted as the rate of change of A along an integral curve of u. Firstly, the term proportional to $\partial A^{i_1 \ldots i_a}_{j_1 \ldots j_b}/\partial x^k$ is simply the derivative of the functions

$A^{i_1 \ldots i_a}_{j_1 \ldots j_b}$ along the curve. The terms proportional to $\partial u^k / \partial x^l$ account for the change of the basis elements $\partial/\partial x^i, dx^j$, which is computed by considering the flow of an infinitesimal line segment along the curve. For small values of t, the curve has the Taylor expansion $x^i(t) = x^i(0) + u^i(x^i(0))t + O(t^2)$. The rate of change of the basis element dx^i is therefore

$$\frac{\partial}{\partial t}\bigg|_{t=0} dx^i(t) = du^i(x(0)) = \frac{\partial u^i}{\partial x^j}\bigg|_{x=x(0)} dx^j. \tag{2.3.6}$$

The rate of change of the dual basis element $\partial/\partial x^i$ is then deduced from differentiating the relation $\langle \partial/\partial x^i, dx^j \rangle = \delta^j_i$ in time, giving the formula

$$\frac{\partial}{\partial t}\bigg|_{t=0} \frac{\partial}{\partial x^i} = -\frac{\partial u^j}{\partial x^i}\frac{\partial}{\partial x^j}. \tag{2.3.7}$$

Writing the integral curve definition of the Lie derivative $\mathcal{L}_u A$ of a tensor A in local coordinates then gives

$$\begin{aligned} &\frac{\partial}{\partial t}\bigg|_{t=0} A^{i_1 \ldots i_a}_{j_1 \ldots j_b} \frac{\partial}{\partial x^{i_1}} \otimes \ldots \otimes \frac{\partial}{\partial x^{i_a}} \otimes dx^{j_1} \otimes \ldots \otimes dx^{j_b} \\ &\quad = (\mathcal{L}_u A)^{i_1 \ldots i_a}_{j_1 \ldots j_b} \frac{\partial}{\partial x^{i_1}} \otimes \ldots \otimes \frac{\partial}{\partial x^{i_a}} \otimes dx^{j_1} \otimes \ldots \otimes dx^{j_b}. \end{aligned} \tag{2.3.8}$$

Using (2.3.6, 2.3.7) and the fact that $\partial/\partial t$ obeys the Leibniz rule over tensor products, we see that the two definitions (2.3.4) and (2.3.8) for $\mathcal{L}_u A$ agree.

The integral curves formulation of the Lie derivative has a useful interpretation in fluid dynamics. If u is the velocity field of a fluid, then the operator $\partial_t + \mathcal{L}_u$ can be thought of as a *convected time derivative* on tensors A (Oldroyd) [140], which accounts for both the advection of the tensor components $A^{i_1 \ldots i_a}_{j_1 \ldots j_b}$ and also the stretching of the frame basis $dx^1, \ldots, dx^n$.

We can also give a coordinate-free formulation of the Lie derivative for tensors by considering the one-parameter group of diffeomorphisms generated by u. Let u be a vector field, and write the flow along the integral curve starting at $x \in M$ and at time t as $\Phi_t(x)$. The collection of maps $\Phi_t : M \to M$, parametrised by $t \in \mathbb{R}$, is called the *one-parameter group of diffeomorphisms generated by* u.[7]. Now let v be another vector field. We define the *Lie derivative* of v along u as

$$\mathcal{L}_u v(x) := \lim_{t \to 0} \frac{D\Phi_{-t}|_{\Phi_t(x)} v(\Phi_t(x)) - v(x)}{t}, \tag{2.3.9}$$

[7]For a fixed value of t, it is not always possible to define Φ_t as a diffeomorphism on M, for example when $M = (0, 1)$ and $u = x^2 \frac{\partial}{\partial x}$. A sufficient condition for $\Phi_t : M \to M$ to be well-defined for all $t \in \mathbb{R}$ is that the support of u is compact. However, in local computations, we can always multiply to u a compactly supported smooth bump function ρ that has constant value 1 on the relevant coordinate neighbourhood.

where $D\Phi_{-t}|_{\Phi_t(x)}$: $T_{\Phi_t(x)}M \to T_x(M)$ is the derivative map (or Jacobian) of $\Phi_{-t} : M \to M$ at $\Phi_t(x)$. The Lie derivative of tensors is defined similarly to (2.3.9): let $D^a_b\Phi_{-t}|_{\Phi_t(x)}$: $(\otimes^a T \otimes \otimes^b T^*)_{\Phi_t(x)}M \to (\otimes^a T \otimes \otimes^b T^*)_x(M)$ be the multilinear extension of the derivative map $D\Phi_{-t}$ to the space tensors of rank (a, b). This means that $D^a_b\Phi_{-t}$ acts by the negative adjoint on dual vectors (i.e. when $(a, b) = (0, 1)$) and that it obeys the Leibniz rule over tensor products. The *Lie derivative* of a rank (a, b) tensor A along the vector field u is defined as

$$\mathcal{L}_u A(x) := \lim_{t\to 0} \frac{D^a_b\Phi_{-t}|_{\Phi_t(x)}A(\Phi_t(x)) - A(x)}{t}. \tag{2.3.10}$$

Expanding out the right-hand side of (2.3.10) using local coordinates returns the expression (2.3.4).

2.3.3 Semidirect product Lie–Poisson brackets involving tensors

Consider a tensor bundle $(\otimes^a TM)\otimes(\otimes^b T^*M)$. The action of vector fields on its sections by Lie differentiation (section **2.3.2**) induces the semidirect product Lie algebra $\mathfrak{g} = \mathrm{Vect}(M) \ltimes \Gamma((\otimes^a TM)\otimes(\otimes^b T^*M))$. The dual space $\mathfrak{g}^*$ to this Lie algebra is $\mathrm{Vect}(M)^* \times \Gamma((\otimes^b TM)\otimes (\otimes^a T^*M) \otimes \wedge^n T^*M)$, where $\mathrm{Vect}(M)^* = \Gamma(T^*M \otimes \wedge^n T^*M)$ is the space of one form densities, and $\Gamma((\otimes^b TM)\otimes(\otimes^a T^*M)\otimes\wedge^n T^*M)$ is the smooth dual space to $\Gamma((\otimes^a TM)\otimes (\otimes^b T^*M))$. The dual pairing in both cases is given by integration: let $(u, T) = (u^i, T^{i_1\dots i_a}_{j_1\dots j_b})$ be a typical element of $\mathfrak{g}$. A typical element of $\mathfrak{g}^*$ is a pair $(m, S) = (m_i d^n x, S^{j_1\dots j_b}_{i_1\dots i_a} d^n x)$. The dual pairing between $\mathfrak{g}$ and $\mathfrak{g}^*$ is

$$\langle (m, S), (u, T)\rangle = \int_M \left(u^i m_i d^n x + T^{i_1\dots i_a}_{j_1\dots j_b} S^{j_1\dots j_b}_{i_1\dots i_a} d^n x\right). \tag{2.3.11}$$

The $(-)$-Lie–Poisson bracket for suitable functionals $F = F[m, S], G = G[m, S]$ on $\mathfrak{g}^*$ is

$$\{F, G\}_{\mathfrak{g}} = -\left\langle (m, S), \left(\mathcal{L}_{\frac{\delta F}{\delta m}}\frac{\delta G}{\delta m}, \mathcal{L}_{\frac{\delta F}{\delta m}}\frac{\delta G}{\delta S} - \mathcal{L}_{\frac{\delta G}{\delta m}}\frac{\delta F}{\delta S}\right)\right\rangle. \tag{2.3.12}$$

The semidirect product Lie–Poisson bracket (2.3.12) is used extensively in the Hamiltonian formulation of fluid dynamics, magnetohydrodynamics, and complex fluids [69, 78, 79, 94, 127, 128, 138] (see section **2.6**).

2.3.4 Algebra of functions on a symplectic manifold

Let N be a $2n$-dimensional symplectic manifold, with symplectic form ω. The algebra of functions $C^\infty(N)$ is a Lie algebra under the symplectic Poisson bracket. Here we recall its

construction [27]. Let f be a function on N. Its *Hamiltonian vector field* X_f is the unique vector field that solves the pointwise linear equation

$$\iota_{X_f}\omega = df, \tag{2.3.13}$$

where ι denotes the interior product (contraction with the first index). The *symplectic Poisson bracket* or *canonical Poisson bracket* $\{\cdot,\cdot\} : C^\infty(N) \times C^\infty(N) \to C^\infty(N)$ on N is defined as

$$\{f, g\} = -\mathcal{L}_{X_f} g = \mathcal{L}_{X_g} f = \omega(X_f, X_g), \tag{2.3.14}$$

where f and g are functions on N. It is readily checked that this definition of the symplectic Poisson bracket coincides with the one in section **2.1.1** given in terms of the Poisson tensor.

An important example of a $2n$-dimensional symplectic manifold is the cotangent bundle T^*M of an n-dimensional manifold. The points in T^*M are pairs (x, p), where x is a point on M, and $p \in T^*_x M$ is a cotangent vector at x. On a coordinate neighbourhood U of x, there are induced coordinates $(x^1, \ldots, x^n, p_1, \ldots, p_n)$ on T^*U, where x^i are the coordinates of the basepoint x and $p_i = \langle p, \partial/\partial x^i \rangle$ are the components of the cotangent vector p. They are often called *canonical coordinates* in physics.

In canonical coordinates, the symplectic form on T^*M can be written as $\omega = dx^i \wedge dp_i$. The Poisson bracket $\{\cdot,\cdot\}$ associated to ω is precisely the Poisson bracket in classical mechanics: for functions f, g on T^*M, $\{f, g\}$ is given by

$$\{f, g\} = \frac{\partial f}{\partial x^i}\frac{\partial g}{\partial p_i} - \frac{\partial g}{\partial x^i}\frac{\partial f}{\partial p_i}. \tag{2.3.15}$$

The Lie algebra $C^\infty(N)$ has an important bilinear form given by integration. Let $dV = \omega^n/n!$ denote the *symplectic volume form*[8] on N. For example, if N is the cotangent bundle T^*M of an n-dimensional manifold M, then the local expression for dV in canonical coordinates is

$$dV = dx^1 \wedge \ldots \wedge dx^n \wedge dp_1 \wedge \ldots \wedge dp_n. \tag{2.3.16}$$

Consider the following weakly non-degenerate bilinear form

$$(f, g) = \int_N dV\ fg, \quad \text{where } f, g \text{ are functions on } N \text{ with sufficient decay conditions.} \tag{2.3.17}$$

[8]Despite the notation, dV is not necessarily an exact form.

Remark 2.3. One way to make the decay conditions precise is to take an exhaustion of S by compact submanifolds – take a sequence N_k of compact submanifolds with boundary such that $\cup N_k = N$ and $SN_k \subset \mathrm{Int}(N_{k+1})$, where Int denotes the interior of a manifold with boundary. The decay conditions on f can then be phrased in terms of the decay rates of the numerical sequence $\sup_{x \in N_{k+1} \setminus N_k}(|f(x)|)$, and similarly for its derivatives. For example, if N is the cotangent bundle of a compact Riemannian manifold M, then N_k can be taken as the bundle of balls of radius k in T^*M. Note that the space of functions on a non-compact symplectic manifold N that decay rapidly with rapidly decaying derivatives also forms a Lie algebra under the symplectic Poisson bracket; we denote this Lie algebra also by $C^\infty(N)$ under a slight abuse of notation.

The following lemma demonstrates that $(\cdot, \cdot)$ is an invariant bilinear form on the Lie algebra $C^\infty(N)$, therefore making $C^\infty(N)$ into a quadratic Lie algebra (section **2.2.6**). In particular, $(f, \{g, h\}) = (\{f, g\}, h)$ holds for all $f, g, h \in C^\infty(N)$, provided that at least one of f, g, h decays sufficiently rapidly and has sufficiently rapidly decaying derivatives.

Lemma 2.1. *Let f, g be smooth functions on a symplectic manifold N. Let ω denote the symplectic form and $dV = \omega^n/n!$ be the corresponding symplectic volume form. The following statements hold:*

(i) $\{f, g\}\omega^n$ *is an exact* $2n$*-form.*

(ii) Subject to decay conditions on the integrand, $\int_N dV\ \{f, g\} = 0$.

(iii) Subject to decay conditions on the integrand, $\int_N dV\ \{f, g\}h = \int_N dV\ f\{g, h\}$.

This is a slight generalisation of the situation in usual classical mechanics where $N = \mathbb{R}^{2n}$ is the standard phase space, in which case (ii) and (iii) are straightforward results from integration by parts, assuming boundary terms vanish.

Proof. If X_g is the Hamiltonian vector field of the function g, then $\{f, g\} = \mathcal{L}_{X_g} f$, so

$$\{f, g\}\omega^n = \left(\mathcal{L}_{X_g} f\right)\omega^n = \mathcal{L}_{X_g}\left(f\omega^n\right) - f\mathcal{L}_{X_g}\left(\omega^n\right) = \mathcal{L}_{X_g}\left(f\omega^n\right),$$

since $\mathcal{L}_{X_g}\omega = 0$.[9] Applying Cartan's formula, we see that the Lie derivative of a top degree form is exact. This proves (i).

Applying Stokes' theorem to (i) gives (ii). Using (ii), we have

$$0 = \int_N dV\ \{fh, g\} = \int_N dV\ \left(f\{h, g\} + \{f, g\}h\right),$$

which can be rearranged into the identity (iii). □

[9] This is an easy consequence of Cartan's formula and the definition of X_g.

The (+)-Lie–Poisson bracket for functionals $F[f], G[f]$ on the quadratic Lie algebra $C^\infty(N)$ is then

$$\{F,G\}_{C^\infty(N)} = \left(f, \left\{\frac{\delta F}{\delta f}, \frac{\delta G}{\delta f}\right\}\right) = \int_N dV\ f \left\{\frac{\delta F}{\delta f}, \frac{\delta G}{\delta f}\right\}. \tag{2.3.18}$$

2.4 Noncanonical Hamiltonian mechanics

Noncanonical Hamiltonian mechanics is a coordinate-free generalisation to ordinary Hamiltonian mechanics that encompasses many time-reversible systems. The main references are [94, 137, 154].

Let M be a finite-dimensional Poisson manifold. A noncanonical Hamiltonian system on M is an evolution equation governed by a Hamiltonian function $H \in C^\infty(M)$, given as follows. Define the *Hamiltonian vector field* X_H of the function H by

$$(X_H)^i = \Pi^{ij}\partial_j H, \tag{2.4.1}$$

where $\Pi = \Pi^{ij}$ is the Poisson tensor on M. A more coordinate-free definition of the Hamiltonian vector field is that X_H is the unique vector field associated to the function H satisfying

$$\mathcal{L}_{X_H} F = \{F, H\} \tag{2.4.2}$$

for all functions F. When M is a symplectic manifold, definitions (2.4.2) and (2.3.13) for the Hamiltonian vector field are equivalent. We define the *noncanonical Hamiltonian system generated by* H as the flow of X_H. The time evolution of any function F on M is then given by

$$\frac{\partial F}{\partial t} = \mathcal{L}_{X_H} F = \{F, H\}, \tag{2.4.3}$$

where $\{\cdot,\cdot\}$ is the Poisson bracket given by the Poisson tensor Π. If M is an infinite-dimensional Poisson manifold, we formulate noncanonical Hamiltonian mechanics solely on the space of suitable functionals $\mathcal{F}(M)$ on M instead. Let H be a Hamiltonian functional. The noncanonical Hamiltonian system generated by H is a time evolution equation on $\mathcal{F}(M)$ where any functional F evolves by

$$\frac{\partial F}{\partial t} = \{F, H\}. \tag{2.4.4}$$

In many cases, the equation of motion for a point $z \in M$ can be recovered in a weak sense by applying the chain rule:

$$\left\langle \frac{\delta F}{\delta z}, \frac{\partial z}{\partial t} \right\rangle = \left\langle \frac{\delta F}{\delta z}, \Pi \frac{\delta H}{\delta z} \right\rangle, \text{ so } \frac{\partial z}{\partial t} = \Pi \frac{\delta H}{\delta z}, \tag{2.4.5}$$

where $\Pi : T_z^*M \to T_zM$ is the infinite-dimensional analogue of the Poisson tensor. The validity of this formal calculation has to be checked on a case-by-case basis, but we note that it works for affine Poisson brackets (section **2.1.3**), which is sufficient for our purposes.

Let us return to the case where M is a finite-dimensional Poisson manifold. The assignment $f \mapsto X_f$ of functions to their Hamiltonian vector fields is a Lie algebra anti-homomorphism from $C^\infty(M)$ to $\mathrm{Vect}(M)$. Indeed, the Jacobi identity

$$\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0, \tag{2.4.6}$$

where $f, g, h \in C^\infty(M)$, can be manipulated into the following form using (2.4.2)

$$\mathcal{L}_{X_{\{g,h\}}} f = -\mathcal{L}_{X_g}\mathcal{L}_{X_h} f + \mathcal{L}_{X_h}\mathcal{L}_{X_g} f, \tag{2.4.7}$$

which shows that $X_{\{g,h\}} = -[X_g, X_h]$.

2.4.1 Conserved quantities in noncanonical Hamiltonian mechanics

Let M be a Poisson manifold. Consider the noncanonical Hamiltonian system generated by a given Hamiltonian functional $H \in \mathcal{F}(M)$. A *conserved quantity* is a functional F that does not change in time under time evolution:

$$\frac{\partial F}{\partial t} = \{F, H\} = 0. \tag{2.4.8}$$

We identify the set of conserved quantities as the *centraliser* $C(H)$ of the Hamiltonian functional H:

$$C(H) := \{F \in \mathcal{F}(M) : \{F, H\} = 0\}. \tag{2.4.9}$$

The centraliser $C(H)$ is readily checked to be a Poisson subalgebra of $\mathcal{F}(M)$: if J, K are conserved quantities, so are JK and $\{J, K\}$. In particular, Casimir functionals $C \in Cas(M)$ are in the centraliser $C(H)$ for any H.

If J is a conserved quantity of the noncanonical Hamiltonian system generated by H, then the integral curves of X_H are contained within the level surfaces of J. Conversely, the integral curves of X_J are also contained within the level surfaces of H. The flow of X_J is thus a symmetry of the noncanonical Hamiltonian system generated by H.

2.4.2 Available energy and the energy-Casimir method

Given a noncanonical Hamiltonian system on M generated by a Hamiltonian functional H, what can we say about the equilibrium points of such a system? The *energy–Casimir method*

is a tool from which the equilibrium points can be obtained from a variational principle, as the critical points of an *available energy* functional. The main references for this section and section **2.4.3** are [91, 94, 137, 154, 160].

An *equilibrium point* or a *fixed point* of the noncanonical Hamiltonian system on M generated by H is a point $z_e \in M$ such that

$$X_H(z_e) = 0. \tag{2.4.10}$$

This means that the constant curve $z(t) = z_e$ is a solution of the differential equation $\partial z/\partial t = X_H(z)$. Since $X_H = \Pi(\cdot, dH)$, where Π is the Poisson tensor on M, equilibrium points can be equivalently characterised as

$$z_e \text{ is an equilibrium point} \Leftrightarrow dH(z_e) \in \ker\left(\Pi : T^*_{z_e}M \to T_{z_e}M\right). \tag{2.4.11}$$

In canonical Hamiltonian mechanics, Π is the inverse of a symplectic form, so $\Pi : T^*_{z_e}M \to T_{z_e}M$ is always invertible, and so the equilibrium points correspond precisely to critical points of the Hamiltonian H. In noncanonical Hamiltonian mechanics, the condition (2.4.11) becomes much more complicated. In practice, checking condition (2.4.11) is often no simpler than manipulating the equations of motion directly. Nonetheless, we can still find a simpler sufficient condition using Casimir functionals $C \in Cas(M)$. If C is a Casimir functional, then $\{F, C\} = 0$ for all $F \in \mathcal{F}(M)$, so X_C vanishes identically. In particular, if $A = H + C$, then $X_A = X_H$. Thus the noncanonical Hamiltonian system is equivalently generated by A, and $dA(z_e) = 0$ becomes a sufficient condition for z_e to be an equilibrium point. To summarise:

$$d(H + C)(z_e) = 0 \text{ for some } C \in Cas(M) \Rightarrow z_e \text{ is an equilibrium point.} \tag{2.4.12}$$

The method (2.4.12) of finding equilibrium points through extremising $A = H + C$ is known as the *energy-Casimir method*. The functional $A = H + C$ is called an *available energy* or *pseudoenergy* for the equilibrium point z_e. The idea of using available energy to demonstrate stability is as follows: since $dA(z_e) = 0$, we can hope that A is a local minimum at z_e; when A is a local minimum at z_e, points sufficiently close to the z_e will stay close to z_e since the available energy cannot increase. We study this argument more formally in section **2.4.3**.

The energy-Casimir method is closely related to the idea of *dynamical accessibility*, which allows us to think of the critical points of A as the critical points of H subject to kinematic constraints on dynamical accessibility. We say that a point $z_2 \in M$ is *dynamically accessible* from another point $z_1 \in M$ if there exist a sequence of functions $H_1, \ldots H_k \in \mathcal{F}(M)$, such that the point z_2 can be connected with z_1 through a sequence of integral curves

of the respective Hamiltonian vector fields $X_{H_1}, \ldots, X_{H_k}$. Dynamical accessibility is clearly an equivalence relation. Moreover, on a finite-dimensional Poisson manifold M, the set of dynamically accessible points from $z \in M$ is simply the maximal connected symplectic leaf S_z through z. This is because that for any point $z \in M$, there is a sufficiently small neighbourhood U of z such that the points in $S_z \cup U$ are all dynamically accessible from z.

The Casimir functions $C \in Cas(M)$ are always constant along the symplectic leaves. Let us assume that there is a "minimal" set of Casimir functions $C_1, \ldots, C_l$ that distinguishes the maximal connected symplectic leaves completely, i.e. that $C_i(z_1) = C_i(z_2)$ for $i = 1, \ldots l$ if and only if z_1 is dynamically accessible from z_2. The problem of finding critical points of H subject to dynamical accessibility can formulated as a constrained optimisation problem:

$$\text{optimise } H \text{ subject to } C_i = a_i \text{ for } i = 1, \ldots, l, \tag{2.4.13}$$

where $a_1, \ldots, a_l$ are constants corresponding to the particular symplectic leaf. The constrained optimisation problem (2.4.13) can be reformulated as an unconstrained optimisation problem using Lagrange multipliers as long as $dC_1, \ldots dC_l$ are linearly independent at the critical points:

$$\text{optimise } A = H - \sum_{i=1}^{l} \lambda_i \left(C_i - a_i\right), \tag{2.4.14}$$

where $\lambda_1, \ldots \lambda_l$ are Lagrange multipliers. We have thus recovered the available energy as the Lagrangian function for the constrained optimisation problem. If z_e is a critical point of A, then we can think of A as a "true" measure of energy around the point z_e, as we have eliminated the variation of H across the symplectic leaves through the introduction of Lagrange multipliers. However, this interpretation of the available energy is local to a particular equilibrium point. Two different solutions of the unconstrained optimisation problem (2.4.14) can have different values for the Lagrange multipliers λ_i, making it difficult to compare the available energy between two distinct equilibrium points.

It is common in physics to think of the Casimir functionals as *kinematic constraints* to the dynamics on the Poisson manifold M, since the Casimir functionals are constant for any choice of Hamiltonian functional, which is usually the total energy of the system. When one wishes to extend the noncanonical Hamiltonian framework to dissipative systems, it is often worthwhile to consider which kinematic constrains are persevered by the dissipative effects and which are not (see section **2.4.5**).

We conclude this section with the *energy-momentum* method, which is a straightforward extension of the energy-Casimir method for time-dependent solutions that evolve according

to a symmetry transformation [124, 159, 163, 164]. Again consider the noncanonical Hamiltonian system on M generated by H. Suppose that J is a conserved quantity, i.e. that $\{H, J\} = 0$, whose Hamiltonian vector field X_J generates a one-parameter group $\phi_t^J : M \to M$ of symmetry transformations. For example, J could be the total momentum of a continuum system in the x-direction, and X_J generates spatial translations of the continuum system. We are interested in solutions of the noncanonical Hamiltonian system that flows along the integral curves of X_J, i.e.

$$\frac{\partial z}{\partial t} z(t) = X_H(z(t)) = X_J(z(t)). \tag{2.4.15}$$

In the previous example, such solutions would correspond to *travelling waves* that translate along the x-direction at a constant velocity in time. We can find solutions (2.4.15) using the *energy-momentum method*. Consider the *augmented available energy* functional $A = H + C - J$, where C is a Casimir functional. The property (2.4.12) for the critical points of A now becomes

$$d(H + C - J)(z_w) = 0 \text{ for some } C \in Cas(M) \Rightarrow X_H(z_w) = X_J(z_w). \tag{2.4.16}$$

Now let $\phi_t : M \to M$ be one-parameter group of transformations generated by X_H, which gives the time evolution $z(t) = \phi_t(z(0))$ for the noncanonical Hamiltonian system. Since $\{A, H\} = 0$, we have $A = \phi_t^* A$ and hence

$$dA(z) = (D\phi_t)^* dA(\phi_t(z)), \tag{2.4.17}$$

where $(D\phi_t)^* : T^*_{\phi_t(z)} M \to T^*_z M$ is the adjoint linear map of the tangent map $D\phi_t : T_z \to T_{\phi_t(z)}$. In particular, if z_w is a critical point of A, so is $\phi_t(z_w)$, so the condition $X_H = X_J$ holds along the integral curve $\phi_t(z_w)$. Thus $\phi_t(z_w) = \phi_t^J(z_w)$ holds at all times. We have thus derived the *energy-momentum method*, which states that

$$\begin{aligned} &z_w \text{ is a critical point of } A = H + C - J \text{ for some } C \in Cas(M) \\ \Rightarrow\ &z(t) = \phi_t^J(z_w) \text{ is a solution to the system generated by } H. \end{aligned} \tag{2.4.18}$$

The energy-momentum method can also be interpreted in terms of a constrained optimisation problem. By analogy with (2.4.13), let us consider the problem of minimising H subject to all possible physical constraints. We have the kinematic constraints $C_i = a_i$ for $i = 1, \ldots, l$, where C_i are Casimir functionals, as before. Suppose also we have the conserved quantities $J_j \in C(H)$ for $j = 1, \ldots, k$ that are not Casimirs, with prescribed values $J_j = b_j$. The problem of minimising the energy H subject to all these constraints is

$$\text{optimise } H \text{ subject to } C_i = a_i \text{ for } i = 1, \ldots, l \text{ and } J_j = b_j \text{ for } j = 1, \ldots, k, \tag{2.4.19}$$

which can be transformed into an unconstrained optimisation problem using Lagrange multipliers,

$$\text{optimise } A = H - \sum_{i=1}^{l} \lambda_i \left(C_i - a_i\right) - \sum_{j=1}^{k} \mu_j \left(J_j - b_j\right), \tag{2.4.20}$$

where λ_i, μ_j are Lagrange multipliers, provided $dC_1, \ldots, dC_l, dJ_1, \ldots, dJ_k$ are linearly independent at the critical points. The functional A in (2.4.20) then corresponds to an augmented available energy functional $A = H + C - J$ with $J = \sum_{j=1}^{k} \mu_j J_j$.

2.4.3 Lyapunov stability

The *Lyapunov method* of stability, which utilises the presence of a non-increasing available energy function A, is a very general method that applies to dynamical systems on well-behaved topological spaces. Let M be a topological space. A *continuous dynamical system* (or simply dynamical system) on M is a continuous map $\phi : M \times (\mathbb{R}^+ \cup \{0\}) \to M$ such that $\phi(z, 0) = z$ for all $z \in M$. The *flow* of the dynamical system at time t is the map $\phi_t : z \to \phi(z, t)$. A *flow curve* of a dynamical system $z(t)$ is a curve $\mathbb{R}^+ \cup \{0\} \to M$ satisfying $\phi(z(0), t) = z(t)$ for all $t \geq 0$. A *fixed point* (or *equilibrium point*) of the dynamical system ϕ is a point $z_e \in M$ such that $\phi(z_e, t) = z_e$ for all $t \geq 0$. An *invariant subset* is a subset $N \subset M$ such that $\phi_t(N) \subset N$ for all $t \geq 0$. The dynamical system ϕ is called *autonomous* if $\phi(t, \phi(s, z)) = \phi(t + s, z)$ for all $z \in M$ and all $t, s \geq 0$. All noncanonical Hamiltonian systems are autonomous dynamical systems in the topological sense, subject to continuity and the existence of flows for the Hamiltonian vector field X_H for all $t \geq 0$.

An equilibrium point z_e of a dynamical system ϕ on the topological space M is *stable* (or *Lyapunov stable*) if for all neighbourhoods U of z_e, there exists a smaller neighbourhood $V \subset U$ of z_e, such that if $z(t = 0) \in V$ then $z(t) \in U$ for all $t > 0$. Morally, an equilibrium point z_e is stable if all points starting sufficiently close to it stays close to it for all $t > 0$. In applications, the term "nonlinear stability" is sometimes used to distinguish Lyapunov stability with other forms of stability (e.g. linear stability).

Now let M be a metric space, with a distance function $dist : M \times M \to \mathbb{R}^+ \cup \{0\}$. Given a dynamical system ϕ on M, an equilibrium point z_e is *stable* if for all $\epsilon > 0$, there exists some $\delta > 0$ such that if $dist(z_e, z(t = 0)) < \delta$ then $dist(z_e, z(t)) < \epsilon$ for all $t > 0$.

One of the main ways to show that an equilibrium point z_e is stable is to construct a family of bounded invariant neighbourhoods of z_e: for all $\epsilon > 0$, we construct an invariant subset U_ϵ satisfying $B_\delta(z_e) \subset U_\epsilon \subset B_\epsilon(z_e)$ for some $\delta > 0$, where $B_\delta(z_e) = \{z \in M : dist(z, z_e) < \delta\}$ denotes the open ball centred at z_e of radius δ. The *Lyapunov stability*

criterion is a straightforward way to construct these bounded invariant neighbourhoods when an appropriate "energy function" A (sometimes called a *Lyapunov function*) can be found. We state it as follows:

Theorem 2.2 (Lyapunov's stability criterion for equilibrium points)**.** *Let M be a metric space, and let $\phi : M \times (\mathbb{R}^+ \cup \{0\}) \to M$ be an autonomous continuous dynamical system on M. Let z_e be an equilibrium point of the dynamical system. Let $A : M \to \mathbb{R}$ be a continuous function on M such that*

(i) A is a non-increasing function in time i.e. $A(z(t)) \leq A(z(0))$ for all flow curves $z(t)$ of the dynamical system;

(ii) For some $\delta_A > 0$, and some continuous strictly increasing bijection $y : \mathbb{R}^+ \cup \{0\} \to \mathbb{R}^+ \cup \{0\}$ with $y(0) = 0$, the inequality

$$A(z) - A(z_e) \geq y\left(dist(z, z_e)\right) \text{ for all } z \in M \text{ with } dist(z, z_e) \leq \delta_A \tag{2.4.21}$$

holds,

then the equilibrium point z_e is stable.

Proof. Without loss of generality, let $A(z_e) = 0$. Let $0 < \epsilon < \delta_A/2$. The set

$$A^{-1}\left(-\infty, y(\epsilon)\right) = \{z \in M : A(z) < y(\epsilon)\} \tag{2.4.22}$$

is an invariant subset since A is non-increasing, and is open since A is continuous. Consider

$$U_\epsilon := A^{-1}\left(-\infty, y(\epsilon)\right) \cap B_{\delta_A}(z_e). \tag{2.4.23}$$

The inequality (2.4.21) implies that $U_\epsilon \subset B_\epsilon(z_e)$: if $z \in U_\epsilon$, then $A(z) < y(\epsilon)$ and $dist(z, z_e) < \delta_A$, so condition (2.4.21) applies and $y(dist(z, z_e)) \leq A(z) < y(\epsilon)$, therefore $dist(z, z_e) < \epsilon$. Since U_ϵ is open, it contains an open ball $B_\delta(z_e)$ for some $\delta > 0$. We thus have

$$B_\delta(z_e) \subset U_\epsilon \subset B_\epsilon(z_e). \tag{2.4.24}$$

If we can show that U_ϵ is an invariant subset, then z_e is stable. (We do not need to construct U_ϵ for $\epsilon \geq \delta_A/2$ since we can always take a U_ϵ with a smaller ϵ.) Since the dynamical system ϕ is autonomous, it is sufficient to show that there exist some $\tau > 0$ such that $\phi_t(U_\epsilon) \subset U_\epsilon$ for all $0 < t < \tau$, which we demonstrate as follows.

Since $\phi(z, t)$ is continuous in both arguments, there exists some $\tau > 0$ such that $dist(z(t), z(0)) < \delta_A/2$ for all flow curves $z(t)$ and for all $0 < t < \tau$. Let $z(0) \in U_\epsilon$. We

show that $z(t) \in U_\epsilon$ for all $0 < t < \tau$: firstly, since A is non-increasing, $A(z(0)) < y(\epsilon)$ implies $A(z(t)) < y(\epsilon)$; secondly, we have

$$\begin{aligned} dist(z(t), z_e) &\leq dist(z(t), z(0)) + dist(z(0), z_e) \\ &< \frac{\delta_A}{2} + dist(z(0), z_e) \\ &\leq \frac{\delta_A}{2} + y^{-1}\left(A(z(0))\right) \\ &< \frac{\delta_A}{2} + y^{-1}\left(y(\epsilon)\right) \\ &< \frac{\delta_A}{2} + \frac{\delta_A}{2} = \delta_A, \end{aligned} \tag{2.4.25}$$

where we have used the inequality (2.4.21) in the third line of (2.4.25). Hence $z(t) \in B_{\delta_A}(z_e)$ for all $0 < t < \tau$. Therefore U_ϵ is an invariant subset, and the proof is complete. □

2.4.4 Obstructions to the existence of available energy

Let z_e be an equilibrium point of the noncanonical Hamiltonian system on M generated by H. When does an available energy exist? We can analyse this problem on finite-dimensional Poisson manifolds using local Darboux coordinates (2.1.8). Consider the noncanonical Hamiltonian system generated by H on the a finite-dimensional Poisson manifold M. Let $z_e \in M$ be an equilibrium point, and consider a set of local Darboux coordinates $(p_1, \ldots, p_m, q_1, \ldots, q_m, y_1, \ldots, y_l)$ in a coordinate neighbourhood U of z_e, where the coordinates for z_e is 0. Recall that the Poisson tensor Π takes the form

$$\Pi = \sum_{i=1}^{m} \frac{\partial}{\partial q_i} \wedge \frac{\partial}{\partial p_i} + \sum_{i,j=1}^{l} \frac{1}{2} \psi_{ij}(y_1, \ldots, y_l) \frac{\partial}{\partial y_i} \wedge \frac{\partial}{\partial y_j}, \tag{2.4.26}$$

where $\psi_{ij}(y)$ are functions on U depending only on y and satisfying $\psi(0) = 0$. Here we abbreviate the $2m + l$-tuple of Darboux coordinates as (q, p, y).

Let $A = H + C$ be an available energy for the equilibrium point z_e, where C is a Casimir function on M. Since C is a Casimir function, $\partial C/\partial q_i = \partial C/\partial p_i = 0$ for $i = 1, \ldots, m$. The condition $dA = 0$ implies that

$$\frac{\partial H}{\partial q_i} = \frac{\partial H}{\partial p_i} = 0, \quad \frac{\partial H}{\partial y_j} = -\frac{\partial C}{\partial y_j}, \tag{2.4.27}$$

for $i = 1, \ldots, m$, $j = 1, \ldots, l$. We can alternatively state the condition (2.4.27) in terms of Taylor expansions:

$$H(p, q, y) = H(0) - \sum_{j=1}^{l} \lambda_j y_j + O((q, p, y)^2), \quad C(y) = C(0) + \sum_{j=1}^{l} \lambda_j y_j + O(y^2), \tag{2.4.28}$$

where λ_j for $j = 1 \ldots, l$ are some constants.

Conversely, the condition for a point z_e to be an equilibrium point is only that $X_H(z_e) = 0$, which can be stated in Darboux coordinates as

$$\frac{\partial H}{\partial q_i} = \frac{\partial H}{\partial p_i} = 0, \tag{2.4.29}$$

but to find an available energy we need to find a $C \in Cas(M)$ that satisfies $\partial H/\partial y_j = -\partial C/\partial y_j$. There are two main obstructions to solving this problem for arbitrary H. Let us consider U as a Poisson manifold on its own, so that the inclusion $\iota : U \hookrightarrow M$ is a Poisson diffeomorphism with its image. Consider the vector subspace $\ker \Pi(0) = Span(dy_1(0), \ldots, dy_l(0)) \subset T_0^*U$ corresponding to the "non-canonical" directions in U. We state the obstructions as follows:

$$dCas(U)_0 := \{dC(0) : C \in Cas(U)\} \text{ does not span } \ker \Pi(0); \tag{2.4.30}$$

$$\iota^*(Cas(M)) \subsetneq Cas(U), \tag{2.4.31}$$

where $\iota^* : C^\infty(M) \to C^\infty(U)$ is the pullback. The first obstruction (2.4.30) is local in nature, and the second obstruction (2.4.31) is the global problem of whether local Casimir functions on U admit extensions to global Casimir functions on M.

Obstruction (2.4.30) is formulated entirely on the space of local Casimir functions $Cas(U)$. When z_e is a regular point of the Poisson manifold, i.e. when Π has locally constant rank $2m$, the functions $\psi_{ij}(y)$ are identically zero. We then have $Cas(U) = C^\infty(y_1, \ldots, y_l)$, therefore $dCas(U) = \ker \Pi$ and obstruction (2.4.30) does not arise. Since the set of regular points is open and dense on M, obstruction (2.4.30) does not arise generically. Conversely, if

$$\psi_{ij}(y) = \sum_{k=1}^{l} c_{ijk} y_k + O(y^2), \tag{2.4.32}$$

where the c_{ijk} are constants that do not vanish identically, then the Jacobi identity (2.1.1b) implies that the c_{ijk} in fact form the structure constants of a l-dimensional Lie algebra $\mathfrak{g}^l$, with underlying vector space $\ker \Pi(0)$. Any Casimir function $C \in Cas(U)$ has to satisfy

$$0 = \sum_{j=1}^{l} \psi_{ij}(y) \frac{\partial C}{\partial y_j} = \sum_{j,k=1}^{l} c_{ijk} \frac{\partial C}{\partial y_j}(0) y_k + O(y^2), \tag{2.4.33}$$

which means that $dCas(U)_0 \subset \ker(ad : \mathfrak{g}^l \to End(\mathfrak{g}^l)) \subsetneq \mathfrak{g}^l$. In particular, if $\partial H/\partial y \notin \ker(ad)$, then an available energy can never be found. The situation for $\psi_{ij}(y) = O(y^2)$ is considerably more difficult to analyse and we do not attempt it here. For more details on the local structure of Poisson manifolds, see [114, 183].

2.4.5 Double bracket formulation of dissipative systems

There are many ways to extend the noncanonical Hamiltonian formulation to dissipative systems. The most natural way is to introduce a symmetric bracket that represents the dissipative effects. We focus our exposition on a simple mathematical framework where the symmetric bracket mimics the Poisson bracket as closely as possible – for more discussion on other approaches and their interpretations in physics, see [16, 17, 57, 78, 79, 119, 135, 136].

Let M be a Poisson manifold, and $\mathcal{F}(M)$ be the space of suitable functionals on M. By a *symmetric bracket* we mean a positive semidefinite symmetric bilinear form $(\cdot,\cdot) : \mathcal{F}(M) \times \mathcal{F}(M) \to \mathcal{F}(M)$ that satisfies the Leibniz rule on multiplication. In equations, these conditions are

$$(F, F) \geq 0 \tag{2.4.34}$$

$$(FG, H) = F(G, H) + G(F, H) \tag{2.4.35}$$

for all functionals $F, G, H \in \mathcal{F}(M)$. Given an available energy functional $A = H + C$, the *double bracket system* is the dynamical system on M where functionals F on M evolve in time according to

$$\frac{\partial F}{\partial t} = \{F, A\} - \nu(F, A), \tag{2.4.36}$$

where $\nu > 0$ is some real parameter. We think of the limit $\nu \to 0^+$ as the Hamiltonian limit of the dissipative system. On a finite-dimensional Poisson manifold M, such symmetric brackets necessarily come from a symmetric rank-$(2,0)$ tensor $K \in \Gamma(S^2TM)$, such that

$$(f, g) = K(df, dg) = K^{ij} \frac{\partial f}{\partial z^i} \frac{\partial g}{\partial z^j}, \tag{2.4.37}$$

where $f, g \in C^\infty(M)$ and $z^1, \ldots, z^n$ are local coordinates on M. We can write equation of motion for a point $z \in M$ under the double bracket dynamics (2.4.36) as

$$\frac{\partial z^i}{\partial t} = \left(\Pi^{ij} - \nu K^{ij}\right) \frac{\partial A}{\partial z^j}, \tag{2.4.38}$$

where Π is the Poisson tensor. Symmetric brackets defined in terms of a symmetric bilinear form K also exist in infinite dimensions. In this case, the equation of motion for a point $z \in M$ can be recovered in a weak sense by applying the chain rule:

$$\left\langle \frac{\delta F}{\delta z}, \frac{\partial z}{\partial t} \right\rangle = \left\langle \frac{\delta F}{\delta z}, (\Pi - \nu K) \frac{\delta A}{\delta z} \right\rangle \tag{2.4.39}$$

where $\Pi : T_z^*M \to T_zM$ is the infinite-dimensional analogue of the Poisson tensor, and $K : T_z^*M \to T_zM$ is the symmetric bilinear form considered as a linear map $\alpha \to K(\cdot, \alpha)$

from T_z^*M to T_zM. We will henceforth work only with symmetric brackets that are given by a symmetric bilinear from K, even in infinite dimensions.

The first class of physical systems that the double bracket framework can model is *non-equilibrium thermodynamics*. The first law of thermodynamics states that energy is conserved, and the second law of thermodynamics states that entropy is non-decreasing in time[10]. In the following, we give an example of a double bracket formulation for such a closed thermodynamic system. Let the Poisson manifold M be the space of states for the system, where H is the energy functional of a state, and S is an entropy-like quantity for the state. The available energy for this system is then $A = H - S$. We require the symmetric bracket to be chosen such that $(H, F) = 0$ for all $F \in \mathcal{F}(M)$, and also that $S = -C$ is a Casimir functional of the Poisson bracket on m. The double bracket dynamics is then

$$\frac{\partial F}{\partial t} = \{F, H\} + \nu(F, S), \tag{2.4.40}$$

where $F \in \mathcal{F}(M)$ is an arbitrary functional. Observe that $\partial H/\partial t = 0$, and $\partial S/\partial t = \nu(S, S) \geq 0$, with equality if and only if $(S, S)|_{z(t)} = 0$, corresponding respectively to the first and second law of thermodynamics. In particular, a suitable local minimum of A can be shown to be stable using the Lyapunov method (see section **2.4.3**), since $\partial A/\partial t \leq 0$.

For open thermodynamic systems, where the system is allowed to exchange energy with its surroundings, the only requirement is that the available energy A, sometimes called the free energy, is non-increasing in time. There are no additional requirements on the symmetric bracket in this case.

The second class of physical systems that the double bracket framework can model is where the dissipation is *dynamically constrained*. These are dissipative systems on a Poisson manifold M where any state is not allowed to leave its symplectic leaf. Let us foliate M with symplectic leaves[11]. We require the image of $K : T_z^*M \to T_zM$ to be contained in the tangent spaces of the symplectic leaves. In particular, $(C, F) = K(dC, dF) = 0$ for all $F \in \mathcal{F}(M)$ and all $C \in Cas(M)$, since dC is constant along the symplectic leaves of M. The double bracket dynamics generated by the Hamiltonian H is then

$$\frac{\partial F}{\partial t} = \{F, H\} - \nu(F, H), \tag{2.4.41}$$

where $F \in \mathcal{F}(M)$ is an arbitrary functional. Observe now that $\partial H/\partial t = -\nu(H, H) \leq 0$, with equality if and only if $(H, H)|_{z(t)} = 0$, and that any Casimir functional C is a constant

[10]The sign convention that entropy is non-decreasing is common in physics; mathematicians often prefer the opposite sign convention.

[11]In finite dimensions this is always possible, but not necessarily in infinite dimensions [107].

of motion. Rewriting (2.4.41), the equation of motion for a state $z \in M$ is

$$\frac{\partial z}{\partial t} = (\Pi - \nu K)\, dH. \tag{2.4.42}$$

Since the right-hand side of (2.4.42) is a tangent vector along the symplectic leaf through z, the trajectory $z(t)$ does not leave the symplectic leaf through $z(0)$.

The system (2.4.42) always seeks to minimise H subject to the constraints that the Casimirs are constant. The analogy between available energy and dynamically constrained minimisation discussed in section **2.4.2** is thus retained. In real physical systems, the dissipation terms do not necessarily preserve all symplectic leaves, so some Casimir functionals are not constants of motion. In this case, the symmetric bracket should be chosen so that only the appropriate Casimir functionals are preserved. If C is a Casimir functional that is preserved under the dynamics of the particular physical system, then the available energy $A = H - \lambda C$ is still the Lagrangian function of the constrained minimisation problem.

As an example to a double bracket system with dynamically constrained dissipation, let $\mathfrak{g}$ be a quadratic Lie algebra (see section **2.2.6**), whose weakly non-degenerate invariant symmetric bilinear form on B is *positive definite*. Let us equip $\mathfrak{g}$ with the minus Lie–Poisson bracket, and let B be the weakly non-degenerate invariant symmetric bilinear form on $\mathfrak{g}$, which we use to identify $\mathfrak{g}$ and $\mathfrak{g}^*$. Let $H \in \mathcal{F}(\mathfrak{g})$ be a Hamiltonian functional. The equation of motion for a state $X \in \mathfrak{g}$ under noncanonical Hamiltonian system generated by H is

$$\frac{\partial X}{\partial t} = \left[X, \frac{\delta H}{\delta X}\right]. \tag{2.4.43}$$

The tangent space of the symplectic leaf through X is therefore the image of $ad(X) : \mathfrak{g} \to \mathfrak{g}$. Let us construct a symmetric bracket $(\cdot,\cdot)_q$ given by

$$(F, G)_q := B\left(\left[X, \frac{\delta F}{\delta X}\right], \left[X, \frac{\delta G}{\delta X}\right]\right), \tag{2.4.44}$$

where $F, G \in \mathcal{F}(\mathfrak{g})$. The symmetric bracket $(\cdot,\cdot)_q$ is positive semidefinite because B is positive definite. The corresponding tensor $K_X : T_X\mathfrak{g} \times T_X\mathfrak{g} \to \mathbb{R}$ is

$$K_X(Y, Z) = B\left([X, Y], [X, Z]\right), \tag{2.4.45}$$

where $Y, Z \in T_X\mathfrak{g} = \mathfrak{g}$. The image of the map $Y \to K_X(Y,\cdot) = -[X,[X,Y]]$ is in $ad(X)$, so $(\cdot,\cdot)_q$ is a valid symmetric bracket for the dynamically constrained dissipation model. The double bracket system generated by H is then

$$\frac{\partial X}{\partial t} = \left[X, \frac{\delta H}{\delta X}\right] + \nu\left[X, \left[X, \frac{\delta H}{\delta X}\right]\right]. \tag{2.4.46}$$

2.5 Reduction in noncanonical Hamiltonian Mechanics

Given a noncanonical Hamiltonian system on a Poisson manifold M, we can determine the time evolution of all functionals F on M. However, M may have unimportant degrees of freedom. Equivalently, we may only be interested in the time evolution of a certain subset of functionals. There are several ways that one can reduce the degrees of freedom by constructing a reduced noncanonical Hamiltonian system on a smaller Poisson manifold that possesses a certain mathematical relationship with M. The main references are [27, 28, 84, 123, 125, 129, 130, 172].

2.5.1 Reduction via a Poisson map

The simplest form of reduction is via a Poisson map. let M_1 and M_2 be Poisson manifolds, with Poisson brackets $\{\cdot,\cdot\}_1$ and $\{\cdot,\cdot\}_2$ respectively. Recall that a map $J : M_1 \to M_2$ is a *Poisson map* if

$$\{F \circ J, G \circ J\}_1 = \{F, G\}_2 \circ J, \tag{2.5.1}$$

for all functionals $F, G \in \mathcal{F}(M_2)$ (see section **2.1.2**). An important example of a Poisson map is the formal linear adjoint $\phi^* : \mathfrak{g}_2^* \to \mathfrak{g}_1^*$ of a Lie algebra homomorphism $\phi : \mathfrak{g}_1 \to \mathfrak{g}_2$, where $\mathfrak{g}_1^*, \mathfrak{g}_2^*$ are equipped with their respective Lie–Poisson brackets (see section **2.2.1**).

Given a noncanonical Hamiltonian system on M_1 generated by $\tilde{H}$, suppose we are interested in the time evolution of functionals $\tilde{F} \in \mathcal{F}(M_1)$ that depend on $z \in M_1$ only through its image $J[z] \in M_2$, i.e.

$$\tilde{F} = F \circ J \quad \text{for some } F \in \mathcal{F}(M_2). \tag{2.5.2}$$

If the Hamiltonian functional also factors through J i.e. $\tilde{H} \in \mathcal{F}(M_1)$ is of the form

$$\tilde{H} = H \circ J \quad \text{for some } H \in \mathcal{F}(M_2), \tag{2.5.3}$$

then, since J is a Poisson map,

$$\frac{\partial \tilde{F}}{\partial t} = \left\{\tilde{F}, \tilde{H}\right\}_1 = \{F, H\}_2 \circ J, \tag{2.5.4}$$

so we can replace the evolution equation for $\tilde{F}$ with an evolution equation $\partial F/\partial t = \{F, H\}_2$ for F, and forget about M_1 altogether. A Hamiltonian functional that factors through a Poisson map is called *collective* in [84]. The relationship between the Hamiltonian vector fields is

$$DJX_{\tilde{H}}(z) = X_H(J(z)), \tag{2.5.5}$$

where $X_{\tilde{H}}$ is the Hamiltonian vector field of $\tilde{H}$ on M_1, X_H is the Hamiltonian vector field of H on M_2, and $DJ : T_zM_1 \to T_{J(z)}M_2$ is the derivative map of the Poisson map J. So each integral curve of $X_{\tilde{H}}$ is mapped onto an integral curve of X_H.

The problem with this simple type of reduction is that, even if the appropriate reduced Poisson manifold M_2 and the Poisson map $J : M_1 \to M_2$ is found, the original Hamiltonian functional $\tilde{H}$ does not necessarily factor through J. In this case, one has to resort to *approximate reduction*, where one makes physically motivated but otherwise not necessarily controlled approximations to $\tilde{H}$ so that the approximate Hamiltonian $\tilde{H}_{approx}$ factors through J. In many cases, these approximations cannot be justified within the Hamiltonian framework, but the use of the Poisson map ensures that these approximations preserve Hamiltonian properties of the system.

Another common construction for Poisson maps is as follows. Let M_1 be a Poisson manifold, M_2 be a manifold, and $J : M_1 \to M_2$ be a *surjective* map. Then the pullback $J^* : \mathcal{F}(M_2) \to \mathcal{F}(M_1)$ is injective. If we have

$$\{J^*F, J^*H\}_1 \in J^*(\mathcal{F}(M_2)) \quad \text{for all } F, H \in \mathcal{F}(M_2), \tag{2.5.6}$$

then we can define a Poisson bracket $\{\cdot,\cdot\}_2$ on M_2 by requiring

$$J^*\{F, H\}_2 := \{J^*F, J^*H\}_1, \tag{2.5.7}$$

which by the injectivity of J^* defines $\{F, H\}_2$ uniquely. The Poisson bracket $\{\cdot,\cdot\}_2$ automatically satisfies the Leibniz and Jacobi identities (2.1.1a,b) by construction, and $J : M_1 \to M_2$ becomes a Poisson map. An important example of the construction (2.5.6, 2.5.7) is the quotient of a Poisson manifold by a group of Poisson automorphisms ([129], Chapter 10.5). If G is a Lie group acting on M by Poisson automorphisms i.e. the action of each $g \in G$ preserves the Poisson tensor, and if M/G is a manifold, we can identify the space of functionals invariant under the G-action $\mathcal{F}(M)^G$ with the space of functionals on M/G. Since G acts by Poisson automorphisms, $\mathcal{F}(M)^G \subset \mathcal{F}(M)$ is a Poisson subalgebra, so $\mathcal{F}(M/G)$ inherits a Poisson algebra structure from the identification $\mathcal{F}(M)^G \simeq \mathcal{F}(M/G)$. We thus arrive at the situation in (2.5.6, 2.5.7), where the quotient map $\pi : M \to M/G$ plays the role of the surjective map J. A classic example is when $M = T^*G$ is the cotangent bundle of the Lie group G. If we consider the natural left(right)-G action of G on T^*G, the reduced Poisson bracket on $\mathfrak{g}^* = T^*G/G$ is in fact the $+(-)$-Lie–Poisson bracket [30, 128, 129, 130].

So far we have considered the problem of reducing a noncanonical Hamiltonian system on M_1 generated by $\tilde{H}$ via a Poisson map $J : M_1 \to M_2$ to a possibly smaller Poisson manifold M_2, which requires $\tilde{H}$ to be collective i.e. in the image of $J^* : \mathcal{F}(M_2) \to \mathcal{F}(M_1)$. It is also possible to reduce the noncanonical Hamiltonian system with a Poisson map

$I : M_0 \to M_1$, where M_0 is a possibly smaller Poisson manifold. The noncanonical Hamiltonian system on M_0 generated by $H_0 = I^*\tilde{H}$ corresponds to *special solutions* of the more primitive system. Indeed, each integral curve of the Hamiltonian vector field $X_{I^*\tilde{H}}$ on M_0 is mapped onto an integral curve of $X_{\tilde{H}}$ on M_1, since I is a Poisson map. In terms of functionals, the reduction by via Poisson map $I : M_0 \to M_1$ retains only the image $I^*(\mathcal{F}(M_1))$ of the functionals on M_1 i.e. their values on the submanifold $I(M_0) \subset M_1$.

2.5.2 Symmetries and and moment maps

In many physical systems, some excess degrees of freedom are caused by a symmetry in the system. The idea of symmetry in noncanonical Hamiltonian mechanics is expressed in terms of moment maps. Throughout this section, M is a finite-dimensional Poisson manifold, and G is a finite-dimensional Lie group with Lie algebra $\mathfrak{g}$. We will assume some basic background knowledge of Lie groups, which can be found in e.g. [26, 87]. For more detailed expositions, see [27, 28]

Let $\varphi : G \times M \to M$ be a smooth *group action* i.e. φ is a smooth map such that $x \mapsto \varphi(g, x)$ is a diffeomorphism on M, and that $\varphi(g, \varphi(h, x)) = \varphi(gh, x)$ for all $g, h \in G$ and all $x \in M$. We suppress the map φ from the notation and simply write $g \cdot x$ or gx when no confusion can arise. Let $X \in \mathfrak{g}$ and consider the one-parameter group of transformations $\exp(tX) \in G$ for $t \in \mathbb{R}$. Define the *fundamental vector field* $X^\#$ on M associated with X as follows:

$$X^\#(x) := \frac{\partial}{\partial t} \exp(tX)x\big|_{t=0}, \tag{2.5.8}$$

where $x \in M$. The assignment $X \to X^\#$ from $\mathfrak{g}$ to $\mathrm{Vect}(M)$ can be shown to be a Lie algebra anti-homomorphism using the definition of the Lie derivative (2.3.9). Conversely, any Lie algebra anti-homomorphism from $\mathfrak{g}$ to $\mathrm{Vect}(M)$ is called a *Lie algebra action* of $\mathfrak{g}$ on M, or an *infinitesimal group action* of G on M if we think about $\mathfrak{g}$ as the Lie algebra of the Lie group G.

The group action of G on M is called a *Hamiltonian group action* if there exists an *equivariant moment(um) map* $J : M \to \mathfrak{g}^*$. satisfies two conditions: firstly, the Hamiltonian vector field of the real-valued function $J^X : x \mapsto \langle J(x), X\rangle$ is required to be $X^\#$:

$$\mathcal{L}_{X^\#} f = \{f, J^X\}, \tag{2.5.9}$$

for all $f \in C^\infty(M)$; secondly, we require the *equivariance condition*:

$$J(gx) = Ad^*_g J(x), \tag{2.5.10}$$

for all $g \in G$ and all $x \in X$, where Ad_g^* denotes the coadjoint action of g on $J(x) \in \mathfrak{g}^*$. Our convention is that $Ad_g^* : \mathfrak{g}^* \to \mathfrak{g}^*$ is the *inverse* of the linear algebra adjoint of the adjoint action $Ad_g : \mathfrak{g} \to \mathfrak{g}$. Some authors make the distinction between moment maps (maps $J : M \to \mathfrak{g}^*$ that satisfy (2.5.9) but not necessarily (2.5.10)) and equivariant moment maps, but we will henceforth implicitly require all moment maps to be equivariant and drop the distinction.

The first condition (2.5.9) is self-explanatory – the function J^X ought to generate the flow of the one-parameter group $\exp(tX)$. Let us unpack the equivariance condition (2.5.10). Taking the dual pairing of (2.5.10) with an arbitrary $Y \in \mathfrak{g}$ and rearranging gives

$$J^Y(gx) = J^{Ad_{g^{-1}}Y}(x), \tag{2.5.11}$$

for all $g \in G$ and all $x \in M$. An important case is when $g = \exp(tX)$ for some other $X \in \mathfrak{g}$, in which case differentiating (2.5.11) with respect to t at $t = 0$ gives

$$\{J^Y, J^X\} = \mathcal{L}_{X^\#} J^Y = -J^{[X,Y]}, \tag{2.5.12}$$

where $[\cdot, \cdot] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ is the Lie bracket on $\mathfrak{g}$. The first equality comes from the condition (2.5.9). Condition (2.5.12) is called *infinitesimal equivariance*, and it states that the map $X \mapsto J^X$ is a Lie algebra homomorphism from $\mathfrak{g}$ to $(C^\infty(M), \{\cdot, \cdot\})$. Equivariance (2.5.10) implies infinitesimal equivariance (2.5.12); conversely, when G is connected, infinitesimal equivariance (2.5.12) implies equivariance (2.5.10), since the elements $\exp(tX) \in G$ for $X \in \mathfrak{g}$ generate G.

Proposition 2.1. *Let M be a Poisson manifold, and $J : M \to \mathfrak{g}^*$ be a smooth map. Then J is infinitesimally equivariant (i.e. it satisfies (2.5.12)) if and only if J is a Poisson map when $\mathfrak{g}^*$ is equipped with the plus Lie–Poisson bracket.*

Proof. We check this proposition in coordinates. Let $\{\cdot, \cdot\}$ be the Poisson bracket on M, and $\Pi = \Pi^{ij}$ be its Poisson tensor. Let e_a be a basis for $\mathfrak{g}$ and e^a its dual basis for $\mathfrak{g}^*$. We will use the summation convention for the indices $a, b, c, \ldots$ for tensors constructed from $\mathfrak{g}$. In particular, we define the structure constants C^a_{bc} of the Lie algebra by $C^a_{bc} e_a = [e_b, e_c]$. The components of the map J are written as $J_a(x) = J^{e_a}(x)$ in this notation.

The infinitesimal equivariance condition (2.5.12) can be expressed in terms of the basis elements as

$$C^a_{bc} J_a = \{J_b, J_c\}. \tag{2.5.13}$$

On the other hand, the requirement that J is a Poisson map is that, for all $\alpha, \beta \in C^\infty(\mathfrak{g}^*)$, we have

$$J^*\{\alpha, \beta\}_\mathfrak{g} = \{J^*\alpha, J^*\beta\}, \tag{2.5.14}$$

where $J^* : C^\infty(\mathfrak{g}^*) \to C^\infty(M)$ is the pullback by J, and $\{\cdot,\cdot\}_\mathfrak{g}$ is the Lie–Poisson bracket on $\mathfrak{g}^*$. The pullback map J^* is sometimes called the *comoment map*. Let us compute both sides of (2.5.14) in coordinates:

$$m_a C^a_{bc} \frac{\partial \alpha}{\partial m_b}\frac{\partial \beta}{\partial m_c}\bigg|_{m_a = J_a} = \Pi^{ij}\frac{\partial \alpha}{\partial m_b}\frac{\partial J_b}{\partial x^i}\frac{\partial \beta}{\partial m_c}\frac{\partial J_c}{\partial x^j}, \tag{2.5.15}$$

where the chain rule is used to expand the right-hand side of (2.5.14). Since α, β are arbitrary functions, (2.5.15) is equivalent to

$$J_a C^a_{bc} = \Pi^{ij}\frac{\partial J_b}{\partial x^i}\frac{\partial J_c}{\partial x^j}, \tag{2.5.16}$$

which, upon inspection, is equivalent to (2.5.14) when the Poisson bracket is expressed in terms of the Poisson tensor. □

Given a Poisson map $J : M \to \mathfrak{g}^*$, when is it the moment map of a Hamiltonian group action? Composing the chain of assignments $Y \mapsto J^Y \mapsto X_{J^Y}$ for $Y \in \mathfrak{g}$ gives us a Lie algebra anti-homomorphism from $\mathfrak{g}$ to $\mathrm{Vect}(M)$. The problem of integrating Lie algebra actions to group actions has been extensively studied in [142], and we have the following sufficient condition ([142], p.81-82, Corollaries 1 & 2 of Theorem 18):

Theorem 2.3 (Lie–Palais)**.** *Let G be the simply-connected Lie group of the Lie algebra $\mathfrak{g}$. Any Lie algebra action of $\mathfrak{g}$ on a smooth manifold M can be integrated to a unique group action of G on M if the fundamental vector fields of $\mathfrak{g}$ are all compactly supported. In particular, any Lie algebra action of $\mathfrak{g}$ can be integrated to a unique group action of G when M is compact.*

In particular, when the Poisson map $J : M \to \mathfrak{g}^*$ is compactly supported, it is the moment map of the Hamiltonian group action of the simply-connected Lie group G of $\mathfrak{g}$ on M.

We conclude this section with an example of a Poisson map that does not correspond to Hamiltonian group action. Let $\mathbb{R}^2$ be the Poisson manifold with coordinates (x, y) whose Poisson tensor is $\Pi = x(\partial/\partial x) \wedge (\partial/\partial y)$, and let $\mathfrak{n}$ be the 2-dimensional Lie algebra with basis X, Y whose Lie bracket is defined by $[X, Y] = X$. Consider the Poisson map $J : \mathbb{R}^2 \to \mathfrak{n}^*$ given by

$$J^X(x, y) = xy, \quad J^Y(x, y) = y, \tag{2.5.17}$$

which satisfies (2.5.12). However, the flow of J^X is

$$\frac{dx}{dt} = x^2, \quad \frac{dy}{dt} = xy, \tag{2.5.18}$$

which goes to infinity at finite time $x(t=0)^{-1}$ if $x(t=0) > 0$.

2.5.3 Moment maps and Marsden–Weinstein reduction

When a noncanonical Hamiltonian system has a symmetry given by a Lie group G, we can form a reduced Hamiltonian system with $2\dim(G)$ fewer dimensions. This process is called *Marsden–Weinstein reduction*, and we outline it in this section. The main references are [27, 123, 125, 130, 131].

Let G be a Lie group acting on the Poisson manifold M. The group action is *free* on a subset $S \subset M$ if for all $x \in S$, $gx = x$ implies that g is identity element $I \in G$. A function $f \in C^\infty(M)$ is *G-invariant* if $f(gx) = f(x)$ for all $g \in G$. Similarly, a subset $S \in M$ is *G-invariant* if $gS \subset S$ for all $g \in G$. If G is connected, then a function f is G-invariant on M if and only if $\{f, J^X\} = 0$ for all $X \in \mathfrak{g}$. This is the Hamiltonian analogue of *Noether's theorem* in Lagrangian mechanics.

Now consider a Hamiltonian group action by G on M, with moment map $J : M \to \mathfrak{g}^*$. For the rest of this section, we will assume that G is compact to avoid technicalities. To extend the results beyond compact Lie groups, we refer to the original papers [123, 125, 131]. Let $\mu \in \mathfrak{g}^*$ be an Ad^*-invariant element, that is, $Ad^*_g\mu = \mu$ for all $g \in G$. The set $J^{-1}(\mu)$ is then a G-invariant set: if $x \in J^{-1}(\mu)$, then $J(gx) = Ad^*_g J(x) = J(x) = \mu$ by equivariance (2.5.10). Suppose that G acts freely on $J^{-1}(\mu)$. Then the derivative map $DJ_x : T_xM \to T_\mu\mathfrak{g}^*$ is surjective for all $x \in J^{-1}(\mu)$. To see this, let e_a be a basis for $\mathfrak{g}$, and consider their fundamental vector fields $e_a^\#$. Since the action of G is free on $J^{-1}(\mu)$, the $e_a^\#$ must be linearly independent at each $x \in J^{-1}(\mu)$. But we have $e_a^\#(x) = \Pi(\cdot, dJ^{e_a})(x)$, so the covectors $dJ^{e_a}(x)$ must be linearly independent in T^*_xM as well, from which we see that DJ_x is surjective. Therefore, μ is a regular value of J and $J^{-1}(\mu)$ is a manifold by the implicit function theorem. The slice theorem (see Theorem 23.5 and the following Corollaries and discussion in [27]) then implies that $M_{red} = J^{-1}(\mu)/G$ is a manifold, with $\pi : J^{-1}(\mu) \to M_{red}$ being a principal G-bundle.

The *Marsden–Weinstein* reduction theorem states that the manifold M_{red}, commonly known as the *Marsden–Weinstein quotient*, inherits a Poisson bracket $\{\cdot,\cdot\}_{red}$ in a canonical way from M.

Theorem 2.4 (Marsden–Weinstein)**.** *Let M be a Poisson manifold with Poisson bracket $\{\cdot,\cdot\}$. Let G be a compact Lie group acting on M. Let $\mu \in \mathfrak{g}^*$ be an Ad^*-invariant, and*

such that G acts freely on $J^{-1}(\mu)$. Then $\pi : J^{-1}(\mu) \to M_{red}$ is a principal G-bundle, and the base manifold $M_{red} = J^{-1}(\mu)/G$ can be made into a Poisson manifold in a canonical way.

The Poisson bracket $\{\cdot,\cdot\}_{red}$ on M_{red} is described as follows: let f_{red}, h_{red} be functions on M_{red}. Let f be an arbitrary extension of $\pi^* f_{red}$ from $J^{-1}(\mu)$ to M, and similarly h for $\pi_{red}^* h$. Then $\{f,h\}|_{J^{-1}(\mu)}$ is G-invariant, and so defines a function on $M_{red} = J^{-1}(\mu)/G$, which we define to be $\{f,h\}_{red}$.

When M is a symplectic manifold, the Marsden–Weinstein quotient M_{red} is also a symplectic manifold, with symplectic form ω_{red}. It is related to the symplectic form ω on M by the formula $\iota^*\omega = \pi^*\omega_{red}$, where $\iota : J^{-1}(\mu) \hookrightarrow M$ is the inclusion.

Intuitively, the Jacobi identity is the reason why the Poisson bracket $\{f,h\}$ of two G-invariant functions is again G-invariant: if $\{f, J^X\} = 0$ and $\{h, J^X\} = 0$, then $\{\{f,h\}, J^X\} = 0$. We will discuss the algebraic situation in more detail in section **2.5.4**.

Keeping notation as above, consider the noncanonical Hamiltonian system on M generated by H. Any function $f \in C^\infty(M)$ that is G-invariant on $J^{-1}(\mu)$ defines a function f_{red} on M_{red} such that $\pi^* f_{red} = \iota^* f$. In particular, if H is G-invariant, then we can define H_{red} on M_{red} such that $\pi^* H_{red} = \iota^* H$. Since H is G-invariant, $\{J^X, H\} = 0$ for all $X \in \mathfrak{g}$, so the integral curves of X_H lie within $J^{-1}(\mu)$. The Marsden–Weinstein theorem shows that the projection of the integral curves of X_H under $\pi : J^{-1}(\mu) \to M_{red}$ coincides with the integral curves of $X_{H_{red}}$ on M_{red}. The noncanonical Hamiltonian system on M_{red} generated by H_{red} is called the *Marsden–Weinstein reduction* of the original system. The physical significance for Hamiltonian mechanics is that, on an appropriate level set of the conserved quantity J, we can form a reduced Hamiltonian system that forgets the degrees of freedom along the directions of the G-action.

Marsden–Weinstein reduction can also be used to couple two physical systems. Consider two Poisson manifolds $M_1$and M_2 and a Hamiltonian group action by G on both manifolds, with moment maps J_1 and J_2 respectively. Let Π_1 and Π_2 denote the respective Poisson tensors on M_1 and M_2. Now consider the product Poisson manifold $M_1 \times M_2^-$ with Poisson tensor $\Pi_1 - \Pi_2$, where we have suppressed the projection maps from the notation. Then $J_1 - J_2$ is a moment map for the product G-action on $M_1 \times M_2^-$, and we can form the Marsden–Weinstein quotient $(J_1 - J_2)^{-1}(0)/G$ when suitable technical hypotheses are met. In physics, M_1 is often the phase space for matter, M_2 is the phase space for fields, and $J_1 - J_2 = 0$ is a field equation determining the relationship between matter and fields. For example, in [130], M_1 is the phase space for the kinetic theory of charged particles, M_2 is the space of electromagnetic fields, and $J_1 - J_2 = 0$ is Poisson's equation in electrostatics. For more details on such constructions, see [127, 130, 134].

2.5.4 Marsden–Weinstein reduction on Poisson algebras

In this section we explain Marsden–Weinstein reduction for Poisson algebras, where we construct a reduced Poisson algebra A_{red} from a Poisson algebra A under a symmetry. The algebraic picture is detached from the geometrical premise of manifolds, so the constructions are simpler and do not rely on analytical arguments. The obvious limitation of the algebraic picture is that, if A is an algebra of functions on a manifold M, we cannot show that A_{red} is an algebra of functions on some reduced manifold M_{red} without first constructing M_{red} with other methods.

Let A be a Poisson algebra, and $\mathfrak{g}$ be a Lie algebra. A natural notion of (infinitesimal) symmetry on A is a morphism of Poisson algebras $\phi : \mathcal{P}ol(\mathfrak{g}) \to A$. For example, let M be a Poisson manifold, and let G be a Lie group with Lie algebra $\mathfrak{g}$. If G has a Hamiltonian group action on M, then the comoment map J^* of the group action is always a morphism of Poisson algebras.

Suppose the morphism $\phi : \mathcal{P}ol(\mathfrak{g}) \to A$ is injective, so we can identify $\mathcal{P}ol(\mathfrak{g})$ with its image in A under ϕ. Define the *multiplicative ideal generated by* $\mathcal{P}ol(\mathfrak{g})$ to be the set

$$m\left(\mathcal{P}ol(\mathfrak{g})\right) := \{fX : f \in A, X \in \mathcal{P}ol(\mathfrak{g})\}. \tag{2.5.19}$$

The multiplicative ideal $m\left(\mathcal{P}ol(\mathfrak{g})\right)$ is a Poisson subalgebra of A: consider

$$\{fX, gY\} = fg\{X, Y\} + fY\{g, X\} + gX\{f, Y\} + XY\{f, g\}, \tag{2.5.20}$$

where $f, g \in A$ and $X, Y \in \mathcal{P}ol(\mathfrak{g})$. The first term in (2.5.20) belongs to $m\left(\mathcal{P}ol(\mathfrak{g})\right)$ because $\{X, Y\} \in \mathcal{P}ol(\mathfrak{g})$, and the other terms are obviously in $m\left(\mathcal{P}ol(\mathfrak{g})\right)$. However, $m\left(\mathcal{P}ol(\mathfrak{g})\right)$ is not necessarily a Poisson ideal. To form a quotient involving $\mathcal{P}ol(\mathfrak{g})$ in the denominator, we introduce the notion of a *normaliser*: let S be a multiplicative ideal and Poisson subalgebra of the Poisson algebra A. Its *normaliser* $N(S)$ is the set

$$N(S) := \{f \in A : \{f, X\} \in S \text{ for all } X \in S\}. \tag{2.5.21}$$

There are two key properties to the normaliser:

Lemma 2.2. *Let S be a multiplicative ideal and Poisson subalgebra of the Poisson algebra A. Then*

(i) The normaliser $N(S)$ is a Poisson subalgebra of A.

(ii) The set S is a Poisson ideal of $N(S)$.

Proof. (i) Let $f, g \in N(S)$. We need to prove that fg and $\{f, g\}$ are in $N(S)$. Take an arbitrary $X \in S$. The Leibniz identity (2.1.1a) implies that

$$\{fg, X\} = \{f, X\}g + \{g, X\}f. \tag{2.5.22}$$

Note that $\{f, X\}$ and $\{g, X\}$ are elements in S by definition of $N(S)$, so $\{fg, X\} \in S$ by S being a multiplicative ideal. Therefore $fg \in N(S)$.

Similarly, the Jacobi identity (2.1.1b) implies that

$$\{\{f, g\}, X\} = -\{\{g, X\}, f\} - \{\{X, f\}, g\}. \tag{2.5.23}$$

Again, since $\{f, X\}$ and $\{g, X\}$ are elements in S, $\{\{g, X\}, f\}$ and $\{\{X, f\}, g\}$ are elements in S since $\{N(S), S\} \subset S$. Therefore $\{f, g\} \in N(S)$.

(ii) Since S is a Poisson subalgebra, $S \subset N(S)$. S is already a multiplicative ideal in $N(S)$, so we only need to show it is also an ideal with respect to the Poisson bracket. Let $f, g \in N(S)$ and $X \in S$. We need to show that $\{f, X\} \in S$, but that simply comes from the definition of $N(S)$.

□

The *algebraic Marsden–Weinstein quotient* of the Poisson algebra A under the infinitesimal symmetry generated by $\mathfrak{g}$ is the quotient algebra

$$A_{red} := N(m(\mathscr{P}ol(\mathfrak{g})))/m(\mathscr{P}ol(\mathfrak{g})) \tag{2.5.24}$$

Let us explain the connection to the Marsden–Weinstein quotient M_{red} considered in section **2.5.3**. Let $A = C^\infty(M)$ be the algebra of functions on the Poisson manifold M, G be a connected compact Lie group with Lie algebra $\mathfrak{g}$, and $J : M \to \mathfrak{g}^*$ be the moment map for the Hamiltonian group action of G on M. Suppose that G acts freely on $J^{-1}(0)$. Let $\iota : J^{-1}(0) \hookrightarrow M$ be the inclusion, and $\pi : J^{-1}(0) \to M_{red}$ be the projection along the G-fibres. The normaliser $N(m(\mathscr{P}ol(\mathfrak{g}))) \subset A$ should be considered as the space of functions that are G-invariant on $J^{-1}(0)$: let $f \in C^\infty(M)$ and $X \in \mathfrak{g}$. If $\{f, J^X\} = \sum_i g_i J^{Y_i}$ for some $g_i \in A$ and $Y_i \in \mathfrak{g}$, then $\iota^*\{f, J^X\} = 0$, so f is G-invariant on $J^{-1}(0)$. The quotient by $m(\mathscr{P}ol(\mathfrak{g}))$ corresponds to taking the equivalence relation $f \sim g$ if and only if $f - g = 0$ on $J^{-1}(0)$; that is, f and g are equal on $J^{-1}(0)$ but are arbitrary outside $J^{-1}(0)$. This is because the multiplicative ideal $m(\mathscr{P}ol(\mathfrak{g}))$ generates the space of functions that vanish on $J^{-1}(0)$. We can thus identify A_{red} and $C^\infty(M_{red})$ as multiplicative algebras, since the multiplicative ideal $m(\mathscr{P}ol(\mathfrak{g}))$ corresponds to the submanifold $J^{-1}(0)$, and restricting to the normaliser $N(m(\mathscr{P}ol(\mathfrak{g})))$ corresponds to imposing G-invariance. Furthermore, the description of the

Poisson bracket on M_{red} coincides with that on A_{red}, as it is the bracket induced from the quotient of the Poisson algebra $N(m(\mathcal{P}ol(\mathfrak{g})))$ by the Poisson ideal $m(\mathcal{P}ol(\mathfrak{g}))$.

The algebraic description of Marsden–Weinstein reduction is useful in contexts where one can more or less construct M_{red} explicitly. This allows one to avoid difficult technicalities in considering non-compact Lie groups or infinite-dimensional spaces in full generality.

2.5.5 Reduction by constructing a new Poisson bracket

There is yet another form of reduction that has been recently popular in plasma physics. In [170, 171, 172], various Hamiltonian "reduced fluid models" for drift kinetics are derived by constructing a new but related Poisson bracket on the space of reduced variables. A similar construction is also used to find reduced descriptions for the one-dimensional Vlasov–Ampére system in [145]. We give a brief summary of the techniques involved. Let M_1 be the Poisson manifold of the more primitive variables, with Poisson bracket $\{\cdot,\cdot\}_1$, M_2 be the space of reduced variables, and $\pi : M_1 \to M_2$ be a surjective submersion.

In these applications, given two functionals F, G on M_2, the Poisson bracket of their pullbacks $\{\pi^*F, \pi^*G\}_1$ cannot be expressed as the pullback of some other functional on M_2. There are excess variables not described by the image $\pi(M_1)$ that appear in the expression of $\{\pi^*F, \pi^*G\}_1$. These excess variables are eliminated by imposing a *closure relation* on M_1, which is an additional functional relationship between the excess variables and reduced variables.

One mathematical way to describe the closure relation is as an embedding $\sigma : M_2 \to M_1$, whose image corresponds to the locus of the closure relation on M_1. We require that $\pi \circ \sigma = \mathrm{id}_2$ is the identity map on M_2. In other words, σ is a section of the fibred manifold $\pi : M_1 \to M_2$. Define a bracket $\{\cdot,\cdot\}_2$ on M_2 by

$$\{F, G\}_2 = \sigma^* \{\pi^*F, \pi^*G\}_1 , \tag{2.5.25}$$

where F and G are arbitrary functionals on M_2. The bracket $\{\cdot,\cdot\}_2$ always satisfies the Leibniz identity (2.1.1a). The Jacobinator (2.1.4) of $\{\cdot,\cdot\}_2$ involves both the second derivative of the map π and the first derivative of the map $\sigma \circ \pi$. If the Jacobinator of $\{\cdot,\cdot\}_2$ happens to be zero, then M_2 becomes a Poisson manifold. (he Jacobi identity for $\{\cdot,\cdot\}_2$ is checked manually in [145, 170, 171]. While $\sigma^*\pi^* = \mathrm{id}_2^*$, the composition $\pi^*\sigma^*$ is not the identity for functionals on M_1. The relation (2.5.25) is not the same as (2.5.1), and in particular π is *not* a Poisson map.

In the applications described in [145, 170, 171], the primitive Hamiltonian $\tilde{H}$ generating the dynamics on M_1 is the pullback of some effective Hamiltonian H on M_2 through π, that is, $\tilde{H} = \pi^* H$. The reduced dynamics is then given by

$$\frac{\partial F}{\partial t} = \{F, H\}_2 = \sigma^* \left\{\pi^* F, \tilde{H}\right\}_1, \tag{2.5.26}$$

so the time derivative of the functional F is the value of $\left\{\pi^* F, \tilde{H}\right\}_1$ restricted on $\sigma(M_2)$. In terms of Hamiltonian vector fields, letting $y \in M_2$, we have from (2.5.25) that

$$X_{\tilde{H}}(y) = D\pi_{\sigma(y)} X_H(\sigma(y)), \tag{2.5.27}$$

where $D\pi_{\sigma(y)} : T_{\sigma(y)} M_1 \to T_y M_2$ is the derivative map of π at $\sigma(y)$. So one can think of the reduced dynamics in this case as the primitive dynamics projected on the constraint surface $\sigma(M_2)$.

2.6 Some common noncanonical Hamiltonian systems

In this section we list some common noncanonical Hamiltonian systems that occur in fluid dynamics and kinetic theory. In the following, M is a connected orientable n-dimensional Riemannian manifold without boundary, with Riemannian metric g_{ij}, Levi-Civita connection ∇_i and volume form $\mu = \sqrt{\det g_{ij}} d^n x$. We will assume that either M is compact or sufficient decay conditions are met in the tensor fields to avoid technicalities. In most applications it suffices to consider the cases $M = \mathbb{R}^n$ or $M = \mathbb{T}^n$ with Riemannian metric $g_{ij} = \delta_{ij}$. The main references are [6, 94, 127, 128, 129, 130, 138].

2.6.1 Basic ideal fluid dynamics

The *compressible Euler equations* describes the time evolution of an ideal fluid in the limit of vanishing viscosity and thermal diffusivity. The *momentum density* $m_i(t, x)$, *mass density* $\rho(t, x)$, and the *entropy density* $s(t, x)$ of the fluid evolves according to

$$\frac{\partial \rho}{\partial t} + \nabla_i(\rho u^i) = 0, \tag{2.6.1a}$$

$$\frac{\partial m_j}{\partial t} + \nabla_i(u^i m_j) = -\nabla_j P(\rho, s), \tag{2.6.1b}$$

$$\frac{\partial s}{\partial t} + \nabla_i(u^i s) = 0, \tag{2.6.1c}$$

where $u^i = g^{ij} m_j / \rho$ is the fluid velocity, and $P(\rho, s)$ is the pressure as determined by an equation of state. The momentum equation (2.6.1b) is sometimes written in terms of u as

$$\frac{\partial u_j}{\partial t} + u^i \nabla_i u_j = -\frac{1}{\rho} \nabla_j P(\rho, s). \tag{2.6.2}$$

If the pressure P does not depend on the entropy density, equations (2.6.1a,2.6.1b) forms a closed set of evolution equations known as the compressible Euler equations with constant entropy. In the following, we show that the compressible Euler equations with or without constant entropy form a noncanonical Hamiltonian system respectively, where the underlying Poisson manifold of each system is a dual space to an appropriate semidirect product Lie algebra.

Consider the semidirect product Lie algebra $\mathfrak{s}_A = \mathrm{Vect}(M) \ltimes C^\infty(M, \mathbb{R}^{A+1})$, where the vector fields $u \in \mathrm{Vect}(M)$ act on the $\mathbb{R}^{A+1}$-valued functions $(g_0(x), \dots, g_A(x)) \in C^\infty(M, \mathbb{R}^{A+1})$ by componentwise Lie differentiation. The semidirect product Lie bracket on $\mathfrak{s}_A$ is

$$\left[(u, (g_0, \dots g_A)), (v, (h_0, \dots h_A))\right]_{\mathfrak{s}_A} = \left([u, v], (\mathcal{L}_u h_0 - \mathcal{L}_v g_0, \dots, \mathcal{L}_u h_A - \mathcal{L}_v g_A)\right). \tag{2.6.3}$$

The dual space $\mathfrak{s}_A^*$ of the Lie algebra $\mathfrak{s}_A$ is $\mathrm{Vect}^*(M) \times \Omega^n(M, \mathbb{R}^{A+1})$, where $\mathrm{Vect}^*(M) = \Gamma(T^*M \otimes \wedge^n T^*M)$ is the space of 1-form densities on M, and $\Omega^n(M, \mathbb{R}^{A+1})$ is the space of $\mathbb{R}^{A+1}$-valued volume forms on M, which we can also think of as the space of $A+1$ real-valued volume forms by taking components. A typical element of $\mathfrak{s}_A^*$ can be written as $(m_i dx^i \otimes d^n x, (s_0 d^n x, \dots, s_A d^n x))$, where $m = m_i dx^i \otimes d^n x$ is a 1-form density, and $s_a d^n x$ are top-degree forms for $a = 0, \dots, A$. The dual pairing of $\mathfrak{s}_A^*$ with $\mathfrak{s}_A$ is given by integration:

$$\begin{aligned} &\left\langle \left(m_i dx^i \otimes d^n x, (s_0 d^n x, \dots, s_A d^n x)\right), (u, (g_0, \dots, g_A)) \right\rangle_{\mathfrak{s}_A} \\ &= \int_M d^n x \, \left(m_i u^i + \sum_{a=0}^{A} s_a g_a \right). \end{aligned} \tag{2.6.4}$$

The $(-)$-Lie–Poisson bracket on $\mathfrak{s}_A^*$ is given, for functionals $F, G \in \mathcal{F}(\mathfrak{s}_A^*)$, by

$$\{F, G\}_{\mathfrak{s}_A^*} = -\left\langle m, \left[\frac{\delta F}{\delta m}, \frac{\delta G}{\delta m}\right] \right\rangle_{\mathrm{Vect}(M)} - \sum_{a=0}^{A} \left\langle s_a, \mathcal{L}_{\frac{\delta F}{\delta m}} \frac{\delta G}{\delta s_a} - \mathcal{L}_{\frac{\delta G}{\delta m}} \frac{\delta F}{\delta s_a} \right\rangle_{C^\infty(M)}, \tag{2.6.5}$$

where the angle brackets denote the pairing between the vector space indicated by the subscript and its dual.

2.6.1.1 The compressible Euler equation with non-constant entropy

For $A = 1$, we can interpret $\mathfrak{s}_1^*$ as the configuration space of a compressible fluid with non-constant entropy, where m is the *momentum density*, $s_0 = \rho$ is the *mass density*, and

$s_1 = s$ is the *entropy density*. In terms of the Levi-Civita connection, the Lie–Poisson bracket (2.6.5) on $\mathfrak{s}_1^*$ has the explicit form

$$\begin{aligned}\{F,G\}_{\mathfrak{s}_1^*} = -\int_M m_i \left(\frac{\delta F}{\delta m_j}\nabla_j\frac{\delta G}{\delta m_i} - \frac{\delta G}{\delta m_j}\nabla_j\frac{\delta F}{\delta m_i}\right) \\ + \rho\left(\frac{\delta F}{\delta m_j}\nabla_j\frac{\delta G}{\delta \rho} - \frac{\delta G}{\delta m_j}\nabla_j\frac{\delta F}{\delta \rho}\right) \\ + s\left(\frac{\delta F}{\delta m_j}\nabla_j\frac{\delta G}{\delta s} - \frac{\delta G}{\delta m_j}\nabla_j\frac{\delta F}{\delta s}\right).\end{aligned} \tag{2.6.6}$$

The bracket (2.6.6) is the Poisson bracket for ideal fluids with non-constant entropy [138]. Indeed, the compressible Euler equations with non-constant entropy (2.6.1a-c) is generated by the Hamiltonian functional

$$H_{fluids}[m,\rho,s] = \int_M \left(\frac{|m|^2}{2\rho} + \rho U(\rho,s)\right), \tag{2.6.7}$$

where U is the internal energy density of the fluid as a local function of ρ and s, given by some equation of state. The fluid velocity is $u^i = \delta H/\delta m_i = g^{ij}m_j/\rho$, and the pressure is

$$P(\rho,s) = \rho\frac{\partial(\rho U)}{\partial\rho} + s\frac{\partial(\rho U)}{\partial s} - \rho U(\rho,s). \tag{2.6.8}$$

2.6.1.2 The compressible Euler equation with constant entropy

For $A = 0$, we are left with the momentum density m and the mass density $s_0 = \rho$ of the fluid. In terms of the Levi-Civita connection, the Lie–Poisson bracket (2.6.5) on $\mathfrak{s}_0^*$ has the explicit form

$$\begin{aligned}\{F,G\}_{\mathfrak{s}_0^*} = -\int_M m_i \left(\frac{\delta F}{\delta m_j}\nabla_j\frac{\delta G}{\delta m_i} - \frac{\delta G}{\delta m_j}\nabla_j\frac{\delta F}{\delta m_i}\right) \\ + \rho\left(\frac{\delta F}{\delta m_j}\nabla_j\frac{\delta G}{\delta \rho} - \frac{\delta G}{\delta m_j}\nabla_j\frac{\delta F}{\delta \rho}\right).\end{aligned} \tag{2.6.9}$$

The bracket (2.6.9) is the Poisson bracket for ideal fluids with constant entropy. It is also common to express (2.6.9) in terms of the variables (u,ρ) instead of (m,ρ) where $u = m/\rho$. We distinguish the two sets of variables using the notation $\mathfrak{s}_{0u}^*$ for the space with u instead of m. The Poisson bracket becomes

$$\{F,G\}_{\mathfrak{s}_{0u}^*} = -\int_M \left(\frac{\delta G}{\delta u_i}\frac{\delta F}{\delta u_j}\right)\frac{\nabla_i u_j - \nabla_j u_i}{\rho} + \frac{\delta F}{\delta u_j}\nabla_j\frac{\delta G}{\delta\rho} - \frac{\delta G}{\delta u_j}\nabla_j\frac{\delta F}{\delta\rho}. \tag{2.6.10}$$

The Hamiltonian functional that generates the compressible Euler equations is

$$H_{fluids}[m,\rho] = \int_M \left(\frac{|m|^2}{2\rho} + \rho U(\rho)\right), \tag{2.6.11}$$

where the internal energy density U is now a function of ρ only. For example, the choice

$$U(\rho) = \frac{U_0}{\gamma + 1} \left(\frac{\rho}{\rho_0} \right)^\gamma , \tag{2.6.12}$$

where U_0, ρ_0, γ are constants, gives the evolution equations

$$\frac{\partial \rho}{\partial t} + \nabla_i \left(\rho u^i \right) = 0 \qquad , \tag{2.6.13a}$$

$$\frac{\partial u_j}{\partial t} + u^i \nabla_i u_j = -U_0 \nabla_j \left(\frac{\rho}{\rho_0} \right)^\gamma \qquad , \tag{2.6.13b}$$

which we recognise as the compressible Euler equations of an adiabatic ideal gas with adiabatic index γ.

2.6.1.3 The incompressible Euler equation

The flow of an ideal incompressible fluid is described by the incompressible Euler equation. The fluid velocity $u^j(t, x)$ evolves as

$$\frac{\partial u^j}{\partial t} + u^i \nabla_i u^j = -\nabla_j p, \quad \nabla_i u^i = 0, \tag{2.6.14}$$

where $p(t, x)$ is a scalar field that enforces the incompressibility constraint $\nabla_i u^i = 0$. The incompressible Euler equation (2.6.14) is a noncanonical Hamiltonian system formulated on the dual of a Lie subalgebra of $\mathrm{Vect}(M)$, as we shall explain.

Let $\mathrm{Vect}_\mu(M)$ be the Lie subalgebra of vector fields that preserve the volume form μ:

$$\mathrm{Vect}_\mu(M) := \{ u \in \mathrm{Vect}(M) : \mathcal{L}_u \mu = 0 \}. \tag{2.6.15}$$

This is readily checked to be a Lie subalgebra. In terms of the Levi-Civita connection, the condition $\mathcal{L}_u \mu = 0$ can also be written as $\nabla_i u^i = 0$. The smooth dual space to $\mathrm{Vect}_\mu(M)$ is the space $\Omega^1(M)/d\Omega^0(M)$ of 1-forms modulo exact 1-forms, with a weakly non-degenerate pairing

$$\langle \alpha, u \rangle_{\mathrm{Vect}_\mu(M)} = \int_M \mu \, \alpha_i u^i, \tag{2.6.16}$$

where $\alpha \in \Omega^1(M)/d\Omega^0(M)$ and $u \in \mathrm{Vect}_\mu(M)$. The $(-)$-Lie–Poisson bracket on $\mathrm{Vect}_\mu(M)^* = \Omega^1(M)/d\Omega^0(M)$ is given, for functionals $F, G \in \mathcal{F}(\mathrm{Vect}_\mu(M)^*)$, by

$$\{F, G\}_{\mathrm{Vect}_\mu(M)^*} = -\left\langle \alpha, \left[\frac{\delta F}{\delta \alpha}, \frac{\delta G}{\delta \alpha} \right] \right\rangle_{\mathrm{Vect}_\mu(M)} . \tag{2.6.17}$$

It is common to identify the spaces $\mathrm{Vect}_\mu(M)^*$ and $\mathrm{Vect}_\mu(M)$ using the Riemannian metric in many applications. Denoting the index-lowering operation by $g : T_xM \to T_x^*M$, we define the projection map $\mathbb{P} : \Omega_1(M) \to g(\mathrm{Vect}_\mu(M))$ as follows:

$$\mathbb{P}(w_i) = w_i - \nabla_i f, \quad \text{where } \nabla^i\nabla_i f = \nabla^i w_i. \tag{2.6.18}$$

The map $\mathbb{P}$ is well-defined because functions f that solve $\nabla^i\nabla_i f = \nabla^i w_i$ for a given right-hand side are unique up to an overall additive constant[12]. It is also clear that $\nabla^i\mathbb{P}(w_i) = 0$ for any 1-form w_i. Moreover, we have $\ker\mathbb{P} = d\Omega_0(M)$: if $w = dg$ then the set of solutions to the right-hand side of (2.6.18) is $f = g + C$ for arbitrary constants C, giving $\mathbb{P}(w) = 0$; conversely if $\mathbb{P}(w) = 0$ then $w = df$ with f given by (2.6.18). The map $\mathbb{P}$ is also surjective as the composition $g(\mathrm{Vect}_\mu(M)) \hookrightarrow \Omega_1(M) \xrightarrow{\mathbb{P}} g(\mathrm{Vect}_\mu(M))$ is the identity. We can therefore identify the spaces $g(\mathrm{Vect}_\mu(M))$ and $\mathrm{Vect}_\mu(M)^* = \Omega^1(M)/d\Omega^0(M)$. Under this identification, we can rewrite the Poisson bracket (2.6.17) in terms of $v_i = \mathbb{P}(\alpha_i)$ as

$$\{F, G\}_{\mathrm{Vect}_\mu(M)^*} = -\int_M \mu\, \frac{\delta F}{\delta v_j}\mathbb{P}\left(v_i\left(\nabla_j\frac{\delta G}{\delta v_i}\right) + \nabla_i\left(\frac{\delta G}{\delta v_i}v_j\right)\right). \tag{2.6.19}$$

The incompressible Euler equations is then generated by the Hamiltonian

$$H_\mu[v] = \int_M \mu\, \frac{1}{2}|v|^2, \tag{2.6.20}$$

whose Hamiltonian flow can be checked to be

$$\frac{\partial v_j}{\partial t} = \mathbb{P}\left(-v_i\nabla^i v_j\right), \tag{2.6.21}$$

which coincides with (2.6.14) after defining $u^j = g^{jk}v_j$ and inserting the pressure p as the scalar function that arises in the definition of (2.6.18) of $\mathbb{P}$.

2.6.1.4 Two reductions from compressible hydrodynamics to incompressible hydrodynamics

There are two ways to reduce the Poisson manifold $\mathfrak{s}_0^*$ for compressible hydrodynamics with constant entropy to the Poisson manifold $\mathrm{Vect}_\mu^*(M)$ for incompressible hydrodynamics. The first is by dualising the injective Lie algebra homomorphism $\iota : \mathrm{Vect}_\mu(M) \hookrightarrow \mathfrak{s}_0 = \mathrm{Vect}(M) \ltimes C^\infty(M)$, which gives a Poisson map $\iota^* : \mathfrak{s}_0^* \to \mathrm{Vect}_\mu^*(M)$, given explicitly as

$$\iota^*(m) = \mathbb{P}\left(\frac{m}{\mu}\right), \tag{2.6.22}$$

[12] See e.g. [182] for more details on the Laplace–Beltrami operator on compact connected Riemannian manifolds without boundary.

where we used the identification $\mathrm{Vect}^*_\mu(M) = g(\mathrm{Vect}_\mu(M))$. The second way is to use Marsden–Weinstein reduction (see section **2.5.3**). Consider the abelian Lie group $\mathfrak{t} = C^\infty(M)/\mathbb{R}$ of functions modulo constants, whose Lie algebra is also $\mathfrak{t} = C^\infty(M)/\mathbb{R}$. The group $\mathfrak{t}$ acts on $\mathfrak{s}_0^*$ by

$$m \mapsto m - \rho d\phi, \quad \rho \mapsto \rho, \tag{2.6.23}$$

where $\phi \in \mathfrak{t}$. The action (2.6.23) is in fact a Hamiltonian group action, with moment map $J : \mathfrak{s}_0^* \to \mathfrak{t}^*$ given by

$$J[m, \rho] = \rho - \frac{\int_M \rho}{\int_M \mu}\mu. \tag{2.6.24}$$

Note that the smooth dual space to $\mathfrak{t}$ is the space of volume forms with zero integral over M, with the dual pairing given by integration. Denoting the average $\int_M \rho / \int_M \mu$ by $\bar{\rho}$, the submanifold $J^{-1}(0) \subset \mathfrak{s}_0^*$ corresponds to configurations (m, ρ) where $\rho = \bar{\rho}\mu$, and the Marsden–Weinstein quotient is the space $J^{-1}(0)/\mathfrak{t} = \mathrm{Vect}^*_\mu(M) \times \mathbb{R}\mu$, with typical element

$$\left(\mathbb{P}\left(\frac{m}{\bar{\rho}\mu}\right), \bar{\rho}\mu\right) \in \mathrm{Vect}^*_\mu(M) \times \mathbb{R}\mu, \tag{2.6.25}$$

and the Poisson bracket on $J^{-1}(0)/\mathfrak{t}$ is identical to that for incompressible hydrodynamics (2.6.19), with $\bar{\rho}$ entering only parametrically. The two reductions produce the same image in $\mathrm{Vect}^*_\mu(M)$ up to an overall normalising constant $\bar{\rho}$.

2.6.1.5 Potential flows

We can also reduce the Poisson manifold $\mathfrak{s}_0^*$ for compressible hydrodynamics with constant entropy to that containing only potential flows using a Poisson map. Consider the symplectic vector space $S = \Omega^n(M) \times C^\infty(M)$, with typical element (D, ϕ) where D is a top-degree form and ϕ is a function, with symplectic Poisson bracket

$$\{F, G\}_S = \int_M \frac{\delta F}{\delta D}\frac{\delta G}{\delta \phi} - \frac{\delta G}{\delta D}\frac{\delta F}{\delta \phi}. \tag{2.6.26}$$

Consider the map $\xi : S \to \mathfrak{s}_0^*$, given in components as

$$(m, \rho) = \xi(D, \phi) = (D d\phi, D). \tag{2.6.27}$$

In terms of the variables (u, ρ), the image of ξ is the submanifold of $\mathfrak{s}_0^*$ where the 1-form $u = m/\rho$ is exact. Applying the functional chain rule (2.1.13) then gives, for any functional $F \in \mathcal{F}(\mathfrak{s}_0^*)$, that

$$\frac{\delta F \circ \xi}{\delta D} = \frac{\delta F}{\delta m_i}\nabla_i \phi + \frac{\delta F}{\delta \rho}, \quad \frac{\delta F \circ \xi}{\delta \phi} = -\nabla_j\left(D\frac{\delta F}{\delta m_j}\right), \tag{2.6.28}$$

where $\delta F/\delta m, \delta F/\delta \rho$ are evaluated at the images $(m, \rho) = \xi(D, \phi)$. Substituting (2.6.28) into (2.6.26) then gives

$$\begin{aligned}
\{F \circ \xi, G \circ \xi\}_S = \int_M & -\left(\frac{\delta F}{\delta m_i}\nabla_i\phi + \frac{\delta F}{\delta \rho}\right)\nabla_j\left(D\frac{\delta G}{\delta m_j}\right) \\
& + \left(\frac{\delta G}{\delta m_i}\nabla_i\phi + \frac{\delta G}{\delta \rho}\right)\nabla_j\left(D\frac{\delta F}{\delta m_j}\right) \\
= \int_M & D\left(\frac{\delta G}{\delta m_j}\nabla_j\left(\frac{\delta F}{\delta m_i}\nabla_i\phi\right) - \frac{\delta F}{\delta m_j}\nabla_j\left(\frac{\delta G}{\delta m_i}\nabla_i\phi\right)\right) \\
& + D\left(\frac{\delta G}{\delta m_j}\nabla_j\frac{\delta F}{\delta \rho} - \frac{\delta F}{\delta m_j}\nabla_j\frac{\delta G}{\delta \rho}\right) \\
= \int_M & D\nabla_i\phi\left(\frac{\delta G}{\delta m_j}\nabla_j\frac{\delta F}{\delta m_i} - \frac{\delta F}{\delta m_j}\nabla_j\frac{\delta G}{\delta m_i}\right) \\
& + D\left(\frac{\delta G}{\delta m_j}\nabla_j\frac{\delta F}{\delta \rho} - \frac{\delta F}{\delta m_j}\nabla_j\frac{\delta G}{\delta \rho}\right) \\
= & \{F, G\}_{\mathfrak{s}_0^*} \circ \xi,
\end{aligned} \tag{2.6.29}$$

where we have used the fact that $\nabla_i\nabla_j\phi$ is a symmetric tensor in the second-to-last line of (2.6.29). Thus $\xi : S \to \mathfrak{s}_0^*$ is a Poisson map. We can pullback the compressible fluid Hamiltonian (2.6.11) to S and consider the noncanonical Hamiltonian system generated by

$$\xi^* H_{fluids}[D, \phi] = \int_M D\left(\frac{1}{2}|\nabla\phi|^2 + U(D)\right), \tag{2.6.30}$$

as long as we are only interested in potential flows $m_i/\rho = \nabla_i\phi$.

2.6.2 Ideal magnetohydrodynamics

Ideal compressible and incompressible hydrodynamics are both noncanonical Hamiltonian systems, each formulated on the dual of an appropriate semidirect product Lie algebra. We will focus on the case where M is 3-dimensional. We will ignore the entropy density in this section, but it can be added back without difficulty.

2.6.2.1 Compressible MHD

Consider the semidirect product Lie algebra $\mathfrak{m} = \mathrm{Vect}(M) \ltimes (C^\infty(M) \oplus \Omega^1(M))$, where $\mathrm{Vect}(M)$ acts on $C^\infty(M)$ and $\Omega^1(M)$ by Lie differentiation (see section **2.3.2**). The smooth dual space $\mathfrak{m}^*$ is $\mathrm{Vect}^*(M) \times \Omega^3(M) \times \Omega^2(M)$, with typical element (m, ρ, B), where $B = B_{jk}dx^j \wedge dx^k$ is the 2-form corresponding to the magnetic field. It is also common to consider B as a vector density in $\Gamma(TM \otimes \Lambda^3 T^*M)$, via the canonical isomorphism

$\Omega^1(M) \to \Gamma(TM \otimes \Lambda^3 T^*M)$, given in components as

$$B_{jk} dx^j \wedge dx^k \mapsto B_{[jk}\delta^i_{l]} \frac{\partial}{\partial x^i} \otimes dx^j \wedge dx^k \wedge dx^l = B^i \frac{\partial}{\partial x^i} \otimes d^3x, \tag{2.6.31}$$

where the square brackets denote the antisymmetrisation of indices. The $(-)$-Lie–Poisson bracket on $\mathfrak{m}^*$ is given, for functionals $F, G \in \mathcal{F}(\mathfrak{m}^*)$, by

$$\begin{aligned}\{F, G\}_{\mathfrak{m}^*} = &- \left\langle m, \left[\frac{\delta F}{\delta m}, \frac{\delta G}{\delta m}\right] \right\rangle_{\mathrm{Vect}(M)} - \left\langle \rho, \pounds_{\frac{\delta F}{\delta m}} \frac{\delta G}{\delta \rho} - \pounds_{\frac{\delta G}{\delta m}} \frac{\delta F}{\delta \rho} \right\rangle_{C^\infty(M)} \\ &- \left\langle B, \pounds_{\frac{\delta F}{\delta m}} \frac{\delta G}{\delta B} - \pounds_{\frac{\delta G}{\delta m}} \frac{\delta F}{\delta B} \right\rangle_{\Omega^1(M)},\end{aligned} \tag{2.6.32}$$

where the angle brackets denote the dual pairings in the subscripted spaces. The bracket (2.6.32) can be written as explicitly as

$$\begin{aligned}\{F, G\}_{\mathfrak{m}^*} = -\int_M \; & m_i \left(\frac{\delta F}{\delta m_j} \nabla_j \frac{\delta G}{\delta m_i} - \frac{\delta G}{\delta m_j} \nabla_j \frac{\delta F}{\delta m_i} \right) \\ & + \rho \left(\frac{\delta F}{\delta m_j} \nabla_j \frac{\delta G}{\delta \rho} - \frac{\delta G}{\delta m_j} \nabla_j \frac{\delta F}{\delta \rho} \right) \\ & + B^i \left(\frac{\delta F}{\delta m_j} \nabla_j \frac{\delta G}{\delta B^i} + \frac{\delta G}{\delta B^j} \nabla_i \frac{\delta F}{\delta m_j} - \frac{\delta G}{\delta m_j} \nabla_j \frac{\delta F}{\delta m_i} - \frac{\delta F}{\delta B^j} \nabla_i \frac{\delta G}{\delta m_j} \right),\end{aligned} \tag{2.6.33}$$

where $F, G \in \mathcal{F}(\mathfrak{m}^*)$. Maxwell's equations require that the divergence of the magnetic field is zero, which in geometrical language is either $dB = 0$ when we consider B as a 2-form, or $\nabla_i B^i = 0$ when we consider B as a vector density. The time evolution of B under the noncanonical Hamiltonian system generated by any Hamiltonian H is

$$\frac{\partial B}{\partial t} = -\pounds_{\frac{\delta H}{\delta m}} B, \tag{2.6.34}$$

from which we see that the condition $dB = 0$ is preserved at all times if it is satisfied initially. The submanifold $\mathfrak{m}_{div}$ consisting of configurations (m, ρ, B) with $dB = 0$ is therefore a Poisson submanifold of $\mathfrak{m}$, with the same Poisson bracket (2.6.32).

The Hamiltonian functional that generates the compressible MHD equations is

$$H = \int_M \left(\frac{|m|^2}{2\rho} + \rho U(\rho) + \frac{|B|^2}{2\mu} \right), \tag{2.6.35}$$

where we consider B as a vector density. Indeed, the equations of motion for the Hamiltonian H on $\mathfrak{m}_{div}$ are

$$\frac{\partial \rho}{\partial t} + \nabla_i(\rho u^i) = 0, \tag{2.6.36a}$$

$$\frac{\partial m_j}{\partial t} + \nabla_i(u^i m_j) = -\nabla_j \left(P(\rho) + \frac{|B|^2}{2\mu} \right) + \nabla^i \frac{B_i B_j}{\mu}, \tag{2.6.36b}$$

$$\frac{\partial B^j}{\partial t} + \nabla_i \left(u^i B^j \right) = B^i \nabla_i u^j. \tag{2.6.36c}$$

An important Casimir functional on $\mathfrak{m}_{div}$ is the *magnetic helicity* of the magnetic field. Suppose that M is simply-connected, so that the first and second de Rham cohomology groups vanish: $0 = H^1(M;\mathbb{R}) = H^2(M;\mathbb{R})$ (the second equality follows from Poincaré duality). Then for any exact 2-form B there exists a 1-form A such that $dA = B$, and moreover this A is unique up to gauge transformations of the form $A \mapsto A + d\phi$ where ϕ is an arbitrary function. The magnetic helicity functional is defined as

$$I[B] = \int_M A \wedge B = \int_M A_i B^i, \tag{2.6.37}$$

which can be readily checked to be independent of the gauge transformation $A \mapsto A + d\phi$.

2.6.2.2 Incompressible MHD

Incompressible MHD is formulated on the dual of the semidirect product Lie algebra $\mathfrak{m}_\mu = \mathrm{Vect}_\mu(M) \ltimes \mathrm{Vect}_\mu^*(M)$. The dual space is $\mathfrak{m}_\mu = \mathrm{Vect}_\mu^*(M) \times \mathrm{Vect}_\mu(M)$, with typical element (v, B), where v is the unique member in the equivalence class $\alpha \in \Omega^1(M)/d\Omega^0(M) = \mathrm{Vect}_\mu^*(M)$ satisfying $\nabla^i v_i = 0$ (see section **2.6.1.3**), and $B = B^i \partial/\partial x^i$ is a divergence-free vector field. We consider v to be the incompressible fluid velocity and B to be the magnetic field. Note that the definition of B in the incompressible setting differs from that in the compressible setting by the volume form μ, but we can safely disregard this difference because the volume form is invariant under incompressible fluid motion.

The Poisson bracket on $\mathfrak{m}_\mu^*$ is, for functionals $F, G \in \mathcal{F}(\mathfrak{m}_\mu^*)$,

$$\{F,G\}_{\mathfrak{m}_\mu^*} = -\left\langle v, \left[\frac{\delta F}{\delta v}, \frac{\delta G}{\delta v}\right]\right\rangle_{\mathrm{Vect}_\mu(M)} - \left\langle \pounds_{\frac{\delta F}{\delta v}} \frac{\delta G}{\delta B} - \pounds_{\frac{\delta G}{\delta v}} \frac{\delta F}{\delta B}, B \right\rangle_{\mathrm{Vect}_\mu(M)}, \tag{2.6.38}$$

which also has the explicit form

$$\begin{aligned}\{F,G\}_{\mathfrak{m}_\mu^*} = &-\int_M \mu\, v_j \left(\frac{\delta F}{\delta v_j}\nabla_j \frac{\delta G}{\delta v_i} - \frac{\delta G}{\delta v_j}\nabla_j \frac{\delta F}{\delta v_i}\right) \\ &- \int_M \mu\, B^i \left(\frac{\delta F}{\delta v_j}\nabla_j \frac{\delta G}{\delta B^i} + \frac{\delta G}{\delta B^j}\nabla_i \frac{\delta F}{\delta v_j} - \frac{\delta G}{\delta v_j}\nabla_j \frac{\delta F}{\delta v_i} - \frac{\delta F}{\delta B^j}\nabla_i \frac{\delta G}{\delta v_j}\right).\end{aligned} \tag{2.6.39}$$

If M is simply-connected, the helicity I (2.6.37) can similarly be defined and is a Casimir functional on $\mathfrak{m}_\mu^*$. In the incompressible setting, $\mathfrak{m}_\mu^*$ acquires a new Casimir known as the *cross helicity*

$$\chi[v, B] = \int_M \mu\, v_i B^i, \tag{2.6.40}$$

which, upon closer inspection, is the Casimir associated to the polarisation form on $\mathfrak{m}_\mu = \mathrm{Vect}_\mu(M) \ltimes \mathrm{Vect}_\mu^*(M)$ (see section **2.2.6**).

The Hamiltonian functional

$$H = \int_M \mu \left(\frac{1}{2}|v|^2 + \frac{1}{2}|B|^2 \right) \tag{2.6.41}$$

generates the incompressible MHD equations

$$\frac{\partial v_j}{\partial t} + v^i \nabla_i v_j = -\mathbb{P}\left(v^i \nabla_i v_j - \nabla^i (B_i B_j) \right), \tag{2.6.42a}$$

$$\frac{\partial B^j}{\partial t} + v^i \nabla_i B^j = B^i \nabla_i v^j, \tag{2.6.42b}$$

where $\mathbb{P}$ is the incompressible projection (2.6.18).

2.6.3 Collisionless 1-particle kinetic theory

Kinetic theory is formulated on phase space T^*M. In 1-particle kinetic theory, one considers the 1-particle distribution function $f(x, p, t) \in C^\infty(T^*M)$, which gives the expected phase-space density of particles at any given instant. Several collisionless 1-particle kinetic systems can be formulated as noncanonical Hamiltonian systems on the quadratic Lie algebra $C^\infty(T^*M)$ considered as a Poisson manifold (see section **2.3.4**). We will examine collisionless 1-particle kinetic theory in much greater detail in chapter **4**.

The (+)-Lie–Poisson bracket on $C^\infty(T^*M)$ for functionals $F, G \in \mathcal{F}(C^\infty(T^*M))$ is (cf. (2.3.18))

$$\{F, G\}_{C^\infty(T^*M)} = \int_{T^*M} dV \; f \left\{ \frac{\delta F}{\delta f}, \frac{\delta G}{\delta f} \right\}, \tag{2.6.43}$$

where $\{\cdot, \cdot\}$ is the canonical Poisson bracket (2.3.15) on T^*M, and $dV = \omega^n/n! = d^n x d^n p$ is the symplectic volume form. The space $C^\infty(T^*M)$ has a family of Casimir functionals given by

$$C[f] = \int_{T^*M} dV \; y(f), \tag{2.6.44}$$

where y is an arbitrary real-valued function.

The noncanonical Hamiltonian system on $C^\infty(T^*M)$ generated by the Hamiltonian functional $H[f]$ is then

$$\frac{\partial f}{\partial t} = \left\{ \frac{\delta H}{\delta f}, f \right\}, \tag{2.6.45}$$

which preserves the measures of the sets $f^{-1}((a,b])$ for any $a, b \in \{-\infty\} \cup \mathbb{R} \cup \{+\infty\}$. So the subsets

$$C^\infty(T^*M)_+ = \{f \in C^\infty(T^*M) : f(q,p) > 0 \text{ for all } (q,p) \in T^*M\} \tag{2.6.46a}$$

$$C^\infty(T^*M)_{\geq 0} = \{f \in C^\infty(T^*M) : f(x,p) \geq 0 \text{ for all } (x,p) \in T^*M\}\,, \tag{2.6.46b}$$

are invariant under any Hamiltonian flow. Since phase space densities have to be non-negative, we should consider $C^\infty(T^*M)_{\geq 0}$ as the configuration space for 1-particle distribution functions, but it is sometimes convenient to consider only the strictly positive distribution functions $C^\infty(T^*M)_+$ instead for formal calculations involving expressions such as $\log f$.

For $M = \mathbb{T}^n$ or $\mathbb{R}^n$, choosing the Hamiltonian functional

$$H_{KT}[f] = \int d^n x d^n p \, \frac{|p|^2}{2} f \tag{2.6.47}$$

recovers the collisionless Boltzmann equation

$$\frac{\partial f}{\partial t} + p^i \frac{\partial f}{\partial x^i} = 0 \tag{2.6.48}$$

for a dilute gas. The Vlasov–Poisson equation

$$\frac{\partial f}{\partial t} + p^i \frac{\partial f}{\partial x^i} - \left(e^2 \int d^n x' d^n p' \frac{\partial G(x-x')}{\partial x^i} f(x',p') \right) \frac{\partial f}{\partial p_i} = 0 \tag{2.6.49}$$

for an electrostatic plasma, where e is the nondimensionalised charge of the particles and $G(x-x')$ is the Green's function for the Laplacian $-\nabla^2$ on $\mathbb{T}^n$ or $\mathbb{R}^n$, can be obtained from the Vlasov–Poisson Hamiltonian [94, 130, 197]:

$$H_{VP}[f] = \int d^n x d^n p \, \frac{|p|^2}{2} f(q,p) + \frac{e^2}{2} \int d^n x d^n p d^n x' d^n p' f(x,p) f(x',p') G(x-x'). \tag{2.6.50}$$

The electrostatic potential is given by Poisson's equation in electrostatics

$$-\nabla^2 \varphi(x) = e \int d^n p \; f(x,p) \iff \varphi(x) = e \int d^n x' d^n p' \; f(x',p') G(x-x'). \tag{2.6.51}$$

For a plasma on $\mathbb{T}^n$, we assume that there is a uniformly charged inert background to keep the plasma neutral overall, which modifies Poisson's equation (2.6.51) to

$$-\nabla^2 \varphi(x) = e \left(\int d^n p \; f(x,p) - \frac{1}{\mathrm{vol}(\mathbb{T}^n)} \int d^n x d^n p \; f \right). \tag{2.6.52}$$

The Jeans equation for a self-gravitating stellar system in galactic dynamics can be obtained from a slightly different Hamiltonian [19, 98]

$$H_{SG}[f] = \int d^n x d^n p \, \frac{|p|^2}{2} f(x,p) - \frac{\mathrm{G}}{2} \int d^n x d^n p d^n x' d^n p' f(x,p) f(x',p') G(x-x'), \tag{2.6.53}$$

where G is the nondimensionalised gravitational constant. The Jeans equation is identical to the Vlasov–Poisson equation (2.6.49), except that e^2 has been replaced with $-\mathrm{G}$. The sign difference leads to qualitative differences between the respective solutions of the Vlasov–Poisson and Jeans equations [76]. The self-gravitating Hamiltonian $H_{SG}[f]$ is not bounded from below unlike $H_{KT}[f]$ and $H_{VP}[f]$.

Chapter 3

Double bracket formulation of multibead-chain suspensions

In this chapter we describe an application of noncanonical Hamiltonian mechanics in the theory of polymer suspensions. This chapter is based on the author's work in [41]. The outline of the chapter is as follows:

In section **3.1**, we recall some basic notions in the theory of non-Newtonian fluids, using a suspension of bead-spring pairs as the motivating example. We introduce the concepts of a *kinetic model*, where the suspended bodies are modelled with an ensemble distribution function over their macroscopic and internal degrees of freedom, and a *macroscopic model*, where the suspended bodies are modelled with a set of internal state variables. We also introduce the *closure* problem of reducing kinetic models to macroscopic models, which we illustrate by deriving the upper-convected Maxwell model from the kinetic model for a bead-spring pair suspension [21, 51, 148].

In section **3.2**, we recover the bead-spring pair equations using a double bracket formulation (see section **2.4.5**). The complete lift of vector fields to the tangent bundle is used to construct the relevant the semidirect product Lie–Poisson bracket (see section **2.2**). We generalise this construction to the higher order tangent bundles in section **3.3**, and obtain a double bracket formulation for 3-bead chain suspensions in section **3.4**.

It turns out that the 3-bead chain model has an asymmetric stress tensor. This is due to the bending of the chain in the flow, reflected mathematically by the introduction of second derivatives of the flow field u in the complete lift. In section **3.5**, we explain how this fits in to the theory of *generalised continuum systems* [43, 45, 58, 149, 198], where the internal degrees of freedom possess angular momentum and are allowed to exchange angular momentum with the fluid. The bending of the chains leads to an extra angular momentum flux known as the *couple stress*. This new term supports couple stress boundary layers at

rigid boundaries in various shear flow problems [97, 149, 167, 168], which we investigate in section **3.6**.

We return to the general multibead-chain suspension in section **3.7**. We study the closure property of the kinetic model for the multibead-chain suspension with arbitrary internal energy. We find a highly constraining result suggesting that only Hookean multibead-chains lead to exactly closable models. The resulting exactly closable models are generalisations of the upper-convected Maxwell model to Hookean bead-spring chains instead of Hookean bead-spring pairs.

3.1 Introduction – the upper-convected Maxwell model

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. A typical set of governing equations for an isothermal and compressible non-Newtonian fluid on $\mathbb{R}^n$ is

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x^i}\left(\rho u^i\right) = 0, \tag{3.1.1a}$$

$$\frac{\partial u_j}{\partial t} + u^i \frac{\partial u^j}{\partial x^i} u_j = -\frac{1}{\rho}\frac{\partial P(\rho)}{\partial x^j} + \frac{1}{\rho}\frac{\partial {\sigma_{(v)}}_j^k}{\partial x^k} + \frac{1}{\rho}\mathcal{F}_j, \tag{3.1.1b}$$

where u_j is the fluid velocity field, ρ is the density, $P(\rho)$ is the pressure, ${\sigma_{(v)}}^{kj}$ is the Newtonian viscous stress, and $\mathcal{F}_j$ is the body force exerted on the fluid by the internal degrees of freedom. For an incompressible fluid, one takes ρ to be constant and impose the incompressible constraint $\partial u^i/\partial x^i = 0$ on (3.1.1b). In many cases, the force can be written as the divergence of the *particle-contributed stress* $\mathcal{F}_j = \partial \sigma_j^k / \partial x^k$.

There are two main types of models for the force $\mathcal{F}_j$. The first is the *macroscopic model*, where we postulate that a finite number of time-dependent fields $C^{(1)}(x,t), \ldots, C^{(A)}(x,t)$, known as *internal state variables*, describe the state of the internal structure completely. The governing equations are

$$\mathcal{F}_j = \mathcal{F}_j\left[\rho, u_j, C^{(1)}, \ldots, C^{(A)}\right], \tag{3.1.2a}$$

$$\frac{\partial C^{(A)}}{\partial t} = L^{(A)}\left[\rho, u_j, C^{(1)}, \ldots, C^{(A)}\right]. \tag{3.1.2b}$$

Equations (3.1.1a,b, 3.1.2a,b) combine to form to closed system of partial differential equations for the fluid variables ρ, u_j and the internal state variables $C^{(1)}, \ldots, C^{(A)}$. The other type is the *kinetic* model, where the internal state of the suspended bodies is described by an ensemble *distribution function* $\psi(x,y,t)$, which encodes the number density of bodies

at position x and with internal configuration y. The internal configuration space for y is usually a manifold, and we will later see many examples where (x, y) are the coordinates of a suitable fibre bundle over the domain of the fluid. The governing equations are

$$\mathscr{F}_j = \mathscr{F}_j\left[\rho, u_j, \psi\right], \tag{3.1.3a}$$

$$\frac{\partial \psi}{\partial t} = L\left[\rho, u_j, \psi\right], \tag{3.1.3b}$$

where $\mathscr{F}_j\left[\rho, u_j, \psi\right]$ (3.1.3a) usually depends on ψ through some statistical properties of the internal degrees of freedom in the ensemble, for instance certain y-integrals (or y-moments) of $\psi(x, y, t)$. The process of reducing a kinetic model (3.1.3a,b) to an internal state variable model (3.1.2a,b) is known as a *finite closure*. If no approximation is needed for a finite closure, we call it an exact closure; otherwise we call it an approximate closure.

A familiar example of a kinetic model is a dilute suspension of bead-spring pairs [21, 148]. The internal configuration $y \in \mathbb{R}^n$ is a vector describing the relative displacement of the two beads. The evolution equation for the distribution function $\psi(x, y, t)$ is a *Liouville equation*, or a *Fokker–Planck equation*:

$$\frac{\partial \psi}{\partial t} + \frac{\partial}{\partial x^i}\left(u^i \psi\right) + \frac{\partial}{\partial y^i}\left(\frac{\partial u^i}{\partial x^j} y^j \psi\right) = \frac{2}{\zeta}\frac{\partial}{\partial y_i}\left(\delta^{ij}\frac{\partial E(y)}{\partial y^j}\psi\right) + \frac{k_B T}{\zeta}\left(\nabla_x^2 \psi + 2\nabla_y^2 \psi\right), \tag{3.1.4}$$

where $u^i(x, t)$ is the fluid velocity and $E(y)$ is the internal energy density of the bead-spring pairs. Here ζ is a non-negative real number known as the *mobility parameter* of the bead-spring pairs, and $k_B T$ is the temperature of the suspension. The terms in (3.1.4) involving u correspond to the advection of the bead-spring pairs by the fluid, the term involving $E(y)$ corresponds to the internal relaxation of the bead-spring pairs due to elastic forces, and the terms proportional to $k_B T$ correspond to the effect of stochastic Brownian forces on the bead-spring pairs. The bead-spring pairs in turn exert a stress on the fluid given by

$$\sigma_j^k = -2k_B T \int d^n y\ \psi \delta_j^k + \int d^n y\ y^k \frac{\partial E}{\partial y^j}\psi, \tag{3.1.5}$$

which gives the body force as $\mathscr{F}_j = \partial \sigma_j^k / \partial x^k$. The system (3.1.4, 3.1.5) is an instance of a *kinetic model* for a complex fluid suspension, where the time evolution of the ensemble distribution function $\psi(x, y, t)$ for the internal degrees of freedom is obtained from a Fokker–Planck equation that models the microphysics of the suspended particles.

For a Hookean spring, we have $E(y) = (\kappa/2)\delta_{ij} y^j y^k$ and (3.1.5) becomes

$$\sigma^{jk} = -2k_B T \delta^{jk} \int d^n y\ \psi + \kappa \int d^n y\ y^j y^k \psi = -2k_B T \delta^{jk}\langle 1 \rangle + \kappa \left\langle y^j y^k \right\rangle, \tag{3.1.6a}$$

where $\langle \cdots \rangle = \int d^n y \; \psi \, (\cdots)$. Taking the 1 and $y^j y^k$ moments of (3.1.4) gives a closed set of evolution equations

$$\frac{\partial \langle 1 \rangle}{\partial t} + \frac{\partial}{\partial x^i} \left(u^i \langle 1 \rangle \right) = \frac{k_B T}{\zeta} \nabla_x^2 \langle 1 \rangle \,, \tag{3.1.6b}$$

$$\begin{aligned} \frac{\partial \left\langle y^j y^k \right\rangle}{\partial t} + \frac{\partial}{\partial x^i} \left(u^i \left\langle y^j y^k \right\rangle \right) - \frac{\partial u^j}{\partial x^l} \left\langle y^l y^k \right\rangle - \frac{\partial u^k}{\partial x^l} \left\langle y^j y^l \right\rangle \\ = -\frac{4\kappa}{\zeta} \left\langle y^j y^k \right\rangle + \frac{4 k_B T}{\zeta} \delta^{jk} \langle 1 \rangle + \frac{k_B T}{\zeta} \nabla_x^2 \left\langle y^j y^k \right\rangle . \end{aligned} \tag{3.1.6c}$$

The system (3.1.6a-c) is an instance of a macroscopic model (3.1.2a,b) for a non-Newtonian fluid. We have thus obtained an exact, finite closure of the kinetic model (3.1.4, 3.1.6a) for a Hookean bead-spring pair suspension.

Remark 3.1. The example illustrated above is known as the *upper-convected Maxwell model* in the rheological literature [21, 148]. It is typical to assume that the flow is incompressible and that the spatial density of the bead-spring pairs $n_\psi = \langle 1 \rangle$ is constant. We can then decompose the stress (3.1.6a) as

$$\sigma^{jk} = -n_\psi k_B T \delta^{jk} + \sigma^{jk}_{(1)}, \tag{3.1.7}$$

where $n_\psi k_B T$ is the scalar pressure of a suspension of particles without internal structure, and $\sigma^{jk}_{(1)}$ evolves as

$$\begin{aligned} \frac{\partial \sigma^{jk}_{(1)}}{\partial t} + \frac{\partial}{\partial x^i} \left(u^i \sigma^{jk}_{(1)} \right) - \frac{\partial u^j}{\partial x^l} \sigma^{lk}_{(1)} - \frac{\partial u^k}{\partial x^l} \sigma^{jl}_{(1)} \\ = -\frac{4\kappa}{\zeta} \sigma^{jk}_{(1)} + n_\psi k_B T \left(\frac{\partial u^j}{\partial x^l} \delta^{lk} + \frac{\partial u^k}{\partial x^l} \delta^{jl} \right) + \frac{k_B T}{\zeta} \nabla_x^2 \sigma^{jk}_{(1)}, \end{aligned} \tag{3.1.8}$$

which is the usual upper-convected Maxwell model, with an additional diffusion term $(k_B T/\zeta) \nabla_x^2 \sigma^{jk}_{(1)}$. The diffusion term is usually dropped in rheology using lengthscale arguments.

A crucial observation is that, if we treat the configuration space of the bead-spring pairs as the *tangent bundle* $T\mathbb{R}^n$, the left-hand side of (3.1.4) is the action of the *complete lift* of the vector field $u \in \mathrm{Vect}(\mathbb{R}^n)$ to the tangent bundle. This process can be generalised to multibead-chain suspensions using the complete lift to *higher order tangent bundles*, leading to an analogously constructed advection term that involves higher derivatives of u. We review this construction for bead-spring pairs in section **3.2**, and study the generalisation to multibead chains in section **3.3**.

3.2 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 [78]. The double bracket formulation (see section **2.4.5**) is also considered in order to incorporate dissipative and diffusive effects. We recover the kinetic equation for bead-spring pairs in [21, 148] with this formulation.

3.2.1 Tangent bundles

The configuration space of small bead-spring pairs is most naturally described as a tangent bundle. We recall the construction of tangent bundles using equivalence classes of paths, 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 in this chapter. Consider the space of *smooth paths* on M, i.e. the collection of smooth maps $\alpha : I \to M$, where I is a (fixed) closed interval in $\mathbb{R}$ containing 0 in its interior. This space 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

$$\alpha \overset{(1)}{\sim} \beta \text{ if and only if } \alpha(0) = \beta(0), \text{ and } \alpha'(0) = \beta'(0). \tag{3.2.1}$$

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

$$\alpha^i(0) = \beta^i(0), \qquad \frac{d\alpha^i}{dt}(0) = \frac{d\beta^i}{dt}(0). \tag{3.2.2}$$

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 $\alpha^i(t) = x^i + y^i t + O(t^2)$ that belongs to any given class. The space of all such equivalence classes is called the *tangent bundle* TM of M, which 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.

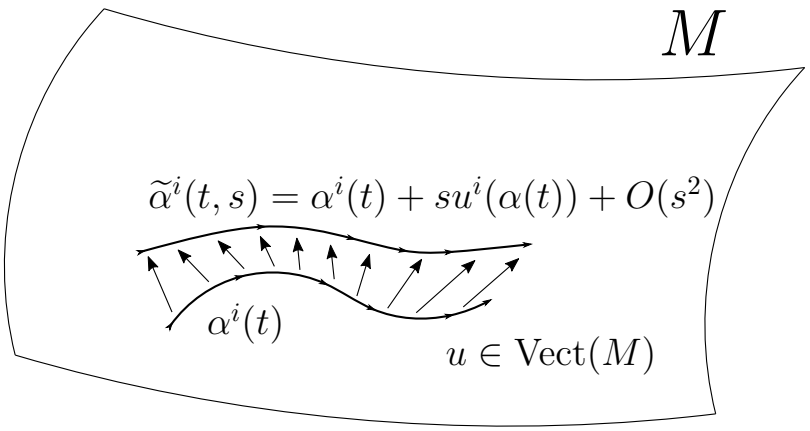


Figure 3.1: The effect of the flow of $u \in \mathrm{Vect}(M)$ on the path $\alpha^i(t)$.

3.2.2 Complete lift of vector fields on M to TM

Since TM is constructed naturally from M, we expect vector fields $u \in \mathrm{Vect}(M)$ 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 $\mathrm{Vect}(M) \ltimes C^\infty(TM)$ 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 $\psi(x,y)d^nxd^ny$, 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 $u \in \mathrm{Vect}(M)$ induces a vector field $u^\# \in \mathrm{Vect}(TM)$, called the *complete lift* or *tangent lift* [192], 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 3.1:

$$\widetilde{\alpha}^i(t,s) = \alpha^i(t) + su^i(\alpha(t)) + O(s^2) \tag{3.2.3}$$

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

$$\widetilde{x}^i(s) = \widetilde{\alpha}^i(0,s), \qquad x^i = \widetilde{x}^i(0), \tag{3.2.4a}$$

$$\widetilde{y}^i(s) = \frac{\partial \widetilde{\alpha}^i}{\partial t}(0,s), \qquad y^i = \widetilde{y}^i(0). \tag{3.2.4b}$$

Then

$$\widetilde{x}^i(s) = \alpha^i(0) + su^i(\alpha(0)) + O(s^2) = x^i + su^i(x) + O(s^2), \tag{3.2.5a}$$

$$\widetilde{y}^i(s) = \frac{d\alpha^i}{dt}(0) + s\frac{\partial u^i}{\partial x^j}(\alpha(0))\frac{d\alpha^j}{dt}(0) + O(s^2) = y^i + s\frac{\partial u^i}{\partial x^j}(x)y^j + O(s^2). \tag{3.2.5b}$$

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

$$\left(u^i(x), \frac{\partial u^i}{\partial x^j}(x) y^j\right). \tag{3.2.6}$$

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

$$u^i(x)\frac{\partial}{\partial x^i} + \frac{\partial u^i}{\partial x^j}(x) y^j \frac{\partial}{\partial y^i}. \tag{3.2.7}$$

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

$$([u, v]_M)^{\#} = \left[u^{\#}, v^{\#}\right]_{TM}, \tag{3.2.8}$$

where the subscripts indicate the spaces on which the vector fields live. A proof sketch can be found in appendix **A.1**. Vector fields $u \in \mathrm{Vect}(M)$ on M can thus act on functions $f \in C^\infty(TM)$ on TM via $f \mapsto u^{\#} \cdot f$, and moreover this action is a Lie algebra representation:

$$\left[u^{\#}, v^{\#}\right]_{TM} \cdot f = u^{\#} \cdot v^{\#} \cdot f - v^{\#} \cdot u^{\#} \cdot f = ([u, v]_M)^{\#} \cdot f. \tag{3.2.9}$$

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

$$\mathfrak{g}_{s1} = \mathrm{Vect}(M) \ltimes (C^\infty(M) \oplus C^\infty(TM)), \tag{3.2.10}$$

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

3.2.3 The Lie–Poisson bracket for bead-spring pair suspensions

Now consider the dual space $\mathfrak{g}_{s1}^*$ of $\mathfrak{g}_{s1} = \mathrm{Vect}(M) \ltimes (C^\infty(M) \oplus C^\infty(TM))$ equipped with the $(-)$-Lie–Poisson bracket. A typical element of $\mathfrak{g}_{s1}^*$ is a triple (m, ρ, ψ), where $m = m_i dx^i \otimes d^n x$ 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 $(-)$-Lie–Poisson bracket for functionals $F[m, \rho, \psi], G[m, \rho, \psi]$ is

$$\begin{aligned}
\{F, G\}_{\mathfrak{g}_{s1}^*} =& -\left\langle m, \left[\frac{\delta F}{\delta m}, \frac{\delta G}{\delta m}\right]\right\rangle_{\mathrm{Vect}(M)} - \left\langle \rho, \frac{\delta F}{\delta m} \cdot \frac{\delta G}{\delta \rho} - \frac{\delta G}{\delta m} \cdot \frac{\delta F}{\delta \rho}\right\rangle_{C^\infty(M)} \\
& - \left\langle \psi, \left(\frac{\delta F}{\delta m}\right)^{\#} \cdot \frac{\delta G}{\delta \psi} - \left(\frac{\delta G}{\delta m}\right)^{\#} \cdot \frac{\delta F}{\delta \psi}\right\rangle_{C^\infty(TM)}, \\
=& \{F, G\}_{fluids} + \{F, G\}_{\psi},
\end{aligned} \tag{3.2.11}$$

where $\{F,G\}_{fluids}$ is the compressible fluid bracket (2.6.6) extended to $\mathfrak{g}_{s1}^*$ by treating the ψ-dependence parametrically, and $\{F,G\}_\psi$ is the new term

$$\{F,G\}_\psi = -\left\langle \psi, \left(\frac{\delta F}{\delta m}\right)^\# \cdot \frac{\delta G}{\delta \psi} - \left(\frac{\delta G}{\delta m}\right)^\# \cdot \frac{\delta F}{\delta \psi} \right\rangle_{C^\infty(TM)}. \tag{3.2.12}$$

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

$$H = H_{fluids}[m,\rho] + H_s[\psi], \tag{3.2.13}$$

where H_{fluids} is the usual ideal compressible fluid Hamiltonian (2.6.11), and $H_s[\psi]$ is the internal free energy of the bead-spring pairs, which is unspecified for now. The coordinate expression of the ψ-term (3.2.12) coincides with that found in [78]. Writing $u^i = \delta H/\delta m_i$, the ψ-term $\{F,H\}_\psi$ is

$$\begin{aligned}
\{F,H\}_\psi =& -\int d^n x d^n y\ \psi \left[\frac{\delta F}{\delta m_i}\frac{\partial}{\partial x^i}\left(\frac{\delta H_s}{\delta \psi}\right) + \frac{\partial}{\partial x^j}\left(\frac{\delta F}{\delta m_i}\right) y^j \frac{\partial}{\partial y^i}\left(\frac{\delta H_s}{\delta \psi}\right)\right] \\
&- \int d^n x d^n y\ \psi \left[-u^i \frac{\partial}{\partial x^i}\left(\frac{\delta F}{\delta \psi}\right) - \frac{\partial u^i}{\partial x^j} y^j \frac{\partial}{\partial y^i}\left(\frac{\delta F}{\delta \psi}\right)\right], \\
=& \left\langle \frac{\delta F}{\delta m_i}, \int d^n y\ \left[-\psi \frac{\partial}{\partial x^i}\left(\frac{\delta H_s}{\delta \psi}\right) + \frac{\partial}{\partial x^j}\left(\psi y^j \frac{\partial}{\partial y^i}\left(\frac{\delta H_s}{\delta \psi}\right)\right)\right]\right\rangle_{\mathrm{Vect}(M)} \\
&+ \left\langle \frac{\delta F}{\delta \psi}, -\frac{\partial}{\partial x^i}\left(u^i \psi\right) - \frac{\partial}{\partial y^i}\left(\frac{\partial u^i}{\partial x^j} y^j \psi\right)\right\rangle_{C^\infty(TM)},
\end{aligned} \tag{3.2.14}$$

from which we obtain the equations of motion for the noncanonical Hamiltonian system generated by H (3.2.13):

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x^i}\left(\rho u^i\right) = 0, \tag{3.2.15a}$$

$$\frac{\partial u_j}{\partial t} + u^i \frac{\partial u^j}{\partial x^i} u_j = -\frac{1}{\rho}\frac{\partial P(\rho)}{\partial x^j} + \frac{1}{\rho}\mathscr{F}_j, \tag{3.2.15b}$$

$$\frac{\partial \psi}{\partial t} + \frac{\partial}{\partial x^i}\left(u^i \psi\right) + \frac{\partial}{\partial y^i}\left(\frac{\partial u^i}{\partial x^j} y^j \psi\right) = 0, \tag{3.2.15c}$$

$$\mathscr{F}_j = \int d^n y\ \left[-\psi \frac{\partial}{\partial x^j}\left(\frac{\delta H_s}{\delta \psi}\right) + \frac{\partial}{\partial x^k}\left(\psi y^k \frac{\partial}{\partial y^j}\left(\frac{\delta H_s}{\delta \psi}\right)\right)\right], \tag{3.2.15d}$$

where $u_j = m_j/\rho$ is the fluid velocity as usual, $P(\rho)$ is the pressure, and $\mathscr{F}_j$ is the extra force on the fluid due to the suspension, which is a y-integral against ψ. For reasonable choices of $H_s[\psi]$, $\mathscr{F}_j$ can be written as the divergence of a stress tensor that depends on *y-moments of* ψ i.e. combinations $\int d^n y\ p(y)\psi$ for polynomials $p(y)$.

Remark 3.2. 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 [21, 148]. If there are no bead-bead interactions and there is no diffusion, the system is Hamiltonian, because the motion of Lagrangian markers 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.

Remark 3.3. The semidirect product Lie–Poisson formulation implements the following physical principles:

- Energy is conserved: $\partial H/\partial t = \{H, H\} = 0$.
- The bead-spring pairs evolve in time as Lagrangian markers, in the sense made precise by the construction of $u^{\#}$ in section **3.2.2**.

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 Poisson bracket depending on ψ. This has been emphasised in [79] and applied in [17] as a uniform way to derive expressions for stress tensors for different complex fluids whose configuration spaces are duals to semidirect product Lie algebras.

3.2.4 The dissipation bracket for bead-spring pairs

To accommodate for irreversible effects in the bead-spring pair suspension, we include an additional symmetric positive semidefinite *dissipation bracket* $(\cdot, \cdot)$ (see section **2.4.5**), such that

$$\frac{\partial F}{\partial t} = \{F, H\} - \frac{1}{\zeta}(F, H), \tag{3.2.16}$$

where $1/\zeta > 0$ is the *mobility* parameter. 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. In the bead-chain

suspension model, we consider the fluid suspension to be held at constant temperature T by an external thermal bath, which makes it open system. The functional H should now be interpreted as the (Helmholtz) free energy. Since the dissipation bracket is positive semidefinite, the free energy is non-increasing in time:

$$\frac{\partial H}{\partial t} = -\frac{1}{\zeta}(H, H) \leq 0. \tag{3.2.17}$$

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

$$ds^2 = \delta_{ij} dx^i dx^j + \delta_{ij} dy^i dy^j, \tag{3.2.18}$$

which 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 [192] (see appendix **A.3**). For any $\lambda > 0$

$$ds^2(\lambda) = \delta_{ij} dx^i dx^j + \lambda \delta_{ij} dy^i dy^j, \tag{3.2.19}$$

is also a valid Riemannian metric on TM. We choose $\lambda = 1/2$ so that the equations we derive later coincide with those in [21, 148]. This is equivalent to rescaling the y-coordinates[1], which leaves the hydrodynamic part of the evolution equation for ψ invariant.

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

$$(F, G) = \left\langle \psi, \widetilde{g}\left(d\left(\frac{\delta F}{\delta \psi}\right), d\left(\frac{\delta G}{\delta \psi}\right)\right)\right\rangle_{C^\infty(TM)}, \tag{3.2.20}$$

where $\widetilde{g}$ is the inverse of the metric (3.2.19) with $\lambda = 1/2$ on TM. The coordinate expression for (F, G) is

$$\begin{aligned}(F, G) &= \int d^n x d^n y\, \psi \left[\delta^{ij} \frac{\partial}{\partial x^i}\left(\frac{\delta F}{\delta \psi}\right) \frac{\partial}{\partial x^j}\left(\frac{\delta G}{\delta \psi}\right) + 2\delta^{ij} \frac{\partial}{\partial y^i}\left(\frac{\delta F}{\delta \psi}\right) \frac{\partial}{\partial y^j}\left(\frac{\delta G}{\delta \psi}\right)\right] \\ &= -\left\langle \frac{\delta F}{\delta \psi}, \frac{\partial}{\partial x^i}\left(\delta^{ij} \psi \frac{\partial}{\partial x^j}\left(\frac{\delta G}{\delta \psi}\right)\right) + 2\frac{\partial}{\partial y^i}\left(\delta^{ij} \psi \frac{\partial}{\partial y^j}\left(\frac{\delta G}{\delta \psi}\right)\right)\right\rangle_{C^\infty(TM)}.\end{aligned} \tag{3.2.21}$$

This type of dissipation bracket coming from a metric allows us to write the evolution of ψ as a Liouville equation $\partial\psi/\partial t + \nabla_x \cdot (\dot{x}\psi) + \nabla_y \cdot (\dot{y}\psi) = 0$, since the extra terms it

[1] 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.

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

$$\begin{aligned}&\frac{\partial\psi}{\partial t} + \frac{\partial}{\partial x^i}\left(u^i\psi\right) + \frac{\partial}{\partial y^i}\left(\frac{\partial u^i}{\partial x^j}y^j\psi\right)\\ &\quad= \frac{1}{\zeta}\left[\frac{\partial}{\partial x^i}\left(\delta^{ij}\psi\frac{\partial}{\partial x^j}\left(\frac{\delta H_s}{\delta\psi}\right)\right) + 2\frac{\partial}{\partial y^i}\left(\delta^{ij}\psi\frac{\partial}{\partial y^j}\left(\frac{\delta H_s}{\delta\psi}\right)\right)\right],\end{aligned} \tag{3.2.22}$$

with the equations for ρ (3.2.15a) and u (3.2.15b) unchanged. The expression for the force $\mathscr{F}_j$ (3.2.15d) on the fluid due to the suspensions is also unchanged. The term $H_s[\psi]$ should now be considered as the free energy of the 2-bead chains. The dissipation bracket (3.2.21) thus relates the non-conservative part of the Fokker–Planck equation and the gradient of the free energy $H_s[\psi]$ using a linear mobility relation.

Remark 3.4. More sophisticated mobility relations can be implemented by modifying the dissipation bracket [17]. 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

$$(F,G)_D = \int d^3x d^3y\ \psi\left[\delta^{ij}\frac{\partial}{\partial x^i}\left(\frac{\delta F}{\delta\psi}\right)\frac{\partial}{\partial x^j}\left(\frac{\delta G}{\delta\psi}\right) + 2D^{ij}(y)\frac{\partial}{\partial y^i}\left(\frac{\delta F}{\delta\psi}\right)\frac{\partial}{\partial y^j}\left(\frac{\delta G}{\delta\psi}\right)\right], \tag{3.2.23}$$

where $D^{ij}(y) = \delta^{ij} + \gamma\Omega^{ij}$ for some parameter γ related to the size of the beads. The quantity $\Omega^{ij} = (|y|^2\delta^{ij} + y^iy^j)/|y|^3$ is the *Oseen–Burgers tensor*, which describes the disturbance flow field around a small sphere in a Stokes flow [108]. 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. In other words, there is no finite and exact closure. Ad hoc techniques such as "pre-averaging" have been used to obtain an effective mobility relation [21], which allows for a particular form of approximate closure.

Remark 3.5. To implement the *Newtonian viscous stress*, we can include an additional term in the dissipation bracket that 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 [16, 17, 57, 135]. 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 chapter, we omit the Newtonian viscous stress term.

3.2.5 The bead-spring pair equations

To conclude this section, we specialise to certain forms of the free energy and recover the usual Fokker–Planck equation (3.1.4) for the bead-spring pair suspension. As before, we postulate a free energy functional of the form $H = H_{fluids}[m, \rho] + H_s[\psi]$, where H_{fluids} is the usual ideal compressible fluid Hamiltonian (2.6.11), and $H_s[\psi]$ is the free energy of the bead-spring pairs, given by

$$H_s[\psi] = \int d^n x d^n y \ \left(E(y)\psi + k_B T \psi \log(\psi)\right), \tag{3.2.24}$$

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

$$U[\psi] = \int d^n x d^n y \ E(y)\psi, \quad S[\psi] = -k_B \int d^n x d^n y \ \psi \log(\psi) \tag{3.2.25}$$

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 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

$$S[\psi] \mapsto S[\psi] + k_B \log(\Lambda) \int d^n x d^n y \ \psi. \tag{3.2.26}$$

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

$$\{F, N\} = -\left\langle \psi, \left(\frac{\delta F}{\delta m}\right)^{\#} \cdot 1 \right\rangle = 0. \tag{3.2.27}$$

Since $d\left(\delta N/\delta\psi\right) = 0$, we also have $(F, N) = 0$ for all functionals F, so the dynamics are unaltered by such rescalings.

Now we can calculate the functional derivative of the free energy $H_s[\psi]$ in (3.2.24):

$$\frac{\delta H_s}{\delta \psi} = E(y) + k_B T \left(\log(\psi) + 1\right). \tag{3.2.28}$$

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

$$\mathcal{F}_j = \frac{\partial}{\partial x^j}\left(-2k_BT\int d^n y\ \psi\right) + \frac{\partial}{\partial x^k}\left(\int d^n y\ y^k \frac{\partial E}{\partial y^j}\psi\right) = \frac{\partial \sigma_j^k}{\partial x^k}, \tag{3.2.29}$$

where

$$\sigma_j^k = -2k_BT\int d^n y\ \psi\delta_j^k + \int d^n y\ y^k \frac{\partial E}{\partial y^j}\psi \tag{3.2.30}$$

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 (3.2.24). The evolution equation (3.2.22) for ψ becomes a *Fokker–Planck equation*:

$$\frac{\partial \psi}{\partial t} + \frac{\partial}{\partial x^i}\left(u^i\psi\right) + \frac{\partial}{\partial y^i}\left(\frac{\partial u^i}{\partial x^j}y^j\psi\right) = \frac{2}{\zeta}\frac{\partial}{\partial y_i}\left(\delta^{ij}\frac{\partial E}{\partial y^j}\psi\right) + \frac{k_BT}{\zeta}\left(\nabla_x^2\psi + 2\nabla_y^2\psi\right). \tag{3.2.31}$$

we have thus recovered the Fokker–Planck equation (3.1.4) of the bead-spring pair suspension from a double bracket formulation.

3.3 Higher order tangent bundles and 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 [109, 141, 192]. This construction enjoys many analogous properties to the tangent bundle considered in section **3.2**, which allows us to consider the advection of distribution functions for multibead-chains using the semidirect product Lie–Poisson formulation.

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

There are better finite-dimensional approximations to the space of all paths $\alpha : I \to M$, 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 $\alpha \overset{(N)}{\sim} \beta$, if and only if the $n(N+1)$ equations hold:

$$\alpha^i(0) = \beta^i(0), \qquad \frac{\mathrm{d}\alpha^i}{\mathrm{d}t}(0) = \frac{\mathrm{d}\beta^i}{\mathrm{d}t}(0), \qquad \frac{\mathrm{d}^N\alpha^i}{\mathrm{d}t^N}(0) = \frac{\mathrm{d}^N\beta^i}{\mathrm{d}t^N}(0). \tag{3.3.1}$$

Each of these equivalence classes is nonempty, since we can construct the local path $\alpha^i(t) = x^i + \sum_{a=1}^N \frac{t^a}{a!}y^i_{(a)} + O(t^{N+1})$ for arbitrary $x^i, y^i_{(1)}, \ldots, y^i_{(N)}$. 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 **3.2.1**. We use $(x^i, y^i_{(1)}, \ldots, y^i_{(N)})$ 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. We can thus consider the space $T^{(N)}M$ as the configuration space of a short $(N+1)$-bead chain living on the domain M.

Remark 3.6. The $(N+1)$-point approximation of a small segment of a smooth path using an N^{th} order Taylor polynomial is a local approximation based at a point. In general, knowing the full Taylor series of a smooth path at one point is not sufficient to determine the value of the path at another arbitrarily close point. For example, the smooth functions $f(t) = \exp(-1/t^2)$ and $g(t) = 0$ have the same Taylor series expansions at $t = 0$, yet $f(t) > g(t)$ for all $t \neq 0$.

3.3.2 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 [192]. Let u be a vector field on M. We construct a vector field $u^{\#}$ on $T^{(N)}M$, called the *complete lift* of u, as follows. Let $\alpha(t)$ be a path on M. The flow of u by a small parameter s deforms the path to $\widetilde{\alpha}(t, s)$ (see figure 3.1), whose components are

$$\widetilde{\alpha}^i(t, s) = \alpha^i(t) + s u^i(\alpha(t)) + O(s^2). \tag{3.3.2}$$

Again, let

$$\begin{aligned} \widetilde{x}^i(s) &= \widetilde{\alpha}^i(0, s), \\ \widetilde{y}^i_{(a)}(s) &= \left.\frac{\partial^a}{\partial t^a}\right|_{t=0} \widetilde{\alpha}^i(t, s), \quad \text{for } a = 1, \ldots, N. \end{aligned} \tag{3.3.3}$$

and denote their values at $s = 0$ as

$$\widetilde{x}^i(0) = x^i, \quad \widetilde{y}^i_{(a)}(0) = y^i_{(a)} \quad \text{for } a = 1, \ldots, N. \tag{3.3.4}$$

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

$$\begin{aligned}
\widetilde{x}^i(s) &= x^i + su^i(x) + O(s^2),\\
\widetilde{y}^i_{(1)}(s) &= y^i_{(1)} + s\frac{\partial u^i}{\partial x^j}(x)y^j_{(1)} + O(s^2),\\
\widetilde{y}^i_{(2)}(s) &= y^i_{(1)} + s\left(\frac{\partial^2 u^i}{\partial x^j x^k}(x)y^j_{(1)}y^k_{(1)} + \frac{\partial u^i}{\partial x^j}(x)y^j_{(2)}\right) + O(s^2),\\
&\vdots\\
\widetilde{y}^i_{(N)}(s) &= y^i_{(N)} + s\left(\frac{\mathrm{d}^N}{\mathrm{d}t^N}u^i(\alpha(t))\right)\bigg|_{t=0} + O(s^2).
\end{aligned} \tag{3.3.5}$$

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

$$u^\#(x, y_{(1)}, \ldots, y_{(N)}) = \left(u^i(\alpha(0)), \frac{\mathrm{d}}{\mathrm{d}t}u^i(\alpha(t))\bigg|_{t=0}, \ldots, \frac{\mathrm{d}^N}{\mathrm{d}t^N}u^i(\alpha(t))\bigg|_{t=0}\right), \tag{3.3.6a}$$

$$\text{where} \quad \alpha^i(t) = x^i + \sum_{a=1}^{N}\frac{t^a}{a!}y^i_{(a)} + O(t^{N+1}). \tag{3.3.6b}$$

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

Crucially, the complete lift of vector fields is a Lie algebra homomorphism $\mathrm{Vect}(M) \to \mathrm{Vect}(T^{(N)}M)$, as

$$([u,v]_M)^\# = \left[u^\#, v^\#\right]_{T^{(N)}M}. \tag{3.3.7}$$

A sketch of proof is given in appendix **A.1**. The action of vector fields u on M on smooth functions f on $T^{(N)}M$ given by $f \mapsto u^\# \cdot f$ is a Lie algebra representation. So we can form the corresponding semidirect product Lie algebra where vector fields u on M acts on functions f on $T^{(N)}M$ by the complete lift.

3.3.3 The Lie–Poisson bracket for multibead chains

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

$$\mathfrak{g}_{sN} = \mathrm{Vect}(M) \ltimes \left(C^\infty(M) \oplus C^\infty(T^{(N)}M)\right). \tag{3.3.8}$$

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 $\psi d^n x d^n y_{(1)} \ldots d^n y_{(N)}$. So the smooth dual space

$\mathfrak{g}_{sN}^*$ can be taken as $\mathrm{Vect}(M)^* \oplus \Omega^n(M) \oplus \Omega^{n(N+1)}(T^{(N)}M)$. A typical element of $\mathfrak{g}_{sN}^*$ is a triple (m, ρ, ψ), where m is the fluid momentum density, ρ is the fluid mass density, and ψ is the distribution function on the configuration space of the $(N+1)$-bead chains. The $(-)$-Lie–Poisson bracket for functionals $F = F[m, \rho, \psi]$ and $G = G[m, \rho, \psi]$ is

$$\begin{aligned}\{F, G\}[m, \rho, \psi] = &- \left\langle m, \left[\frac{\delta F}{\delta m}, \frac{\delta G}{\delta m}\right]\right\rangle - \left\langle \rho, \frac{\delta F}{\delta m} \cdot \frac{\delta G}{\delta \rho} - \frac{\delta G}{\delta m} \cdot \frac{\delta F}{\delta \rho}\right\rangle \\ &- \left\langle \psi, \left(\frac{\delta F}{\delta m}\right)^{\#} \cdot \frac{\delta G}{\delta \psi} - \left(\frac{\delta G}{\delta m}\right)^{\#} \cdot \frac{\delta F}{\delta \psi}\right\rangle \\ = &\{F, G\}_{fluids} + \{F, G\}_{\psi}, \end{aligned} \tag{3.3.9}$$

where $\{F, G\}_{fluids}$ is the compressible fluid bracket (2.6.6) extended to $\mathfrak{g}_{sN}^*$ by treating the ψ-dependence parametrically, and $\{F, G\}_{\psi}$ is the new term

$$\{F, G\}_{\psi} = - \left\langle \psi, \left(\frac{\delta F}{\delta m}\right)^{\#} \cdot \frac{\delta G}{\delta \psi} - \left(\frac{\delta G}{\delta m}\right)^{\#} \cdot \frac{\delta F}{\delta \psi}\right\rangle_{C^\infty(T^{(N)}M)}. \tag{3.3.10}$$

The explicit expression for the complete lifts $(\delta F/\delta m)^{\#}, (\delta G/\delta m)^{\#}$ have to be computed from the defining formulas (3.3.6a,b). We will consider the case $N = 2$ extensively in section **3.4** and the case for arbitrary N in section **3.7**.

3.4 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 3.2. The $(-)$-Lie–Poisson bracket on the dual of the semidirect product Lie algebra $\mathfrak{g}_{s2} = \mathrm{Vect}(M) \ltimes \big(C^\infty(M) \oplus C^\infty(T^{(2)}M)\big)$ is as in (3.3.9, 3.3.10). The explicit expression for

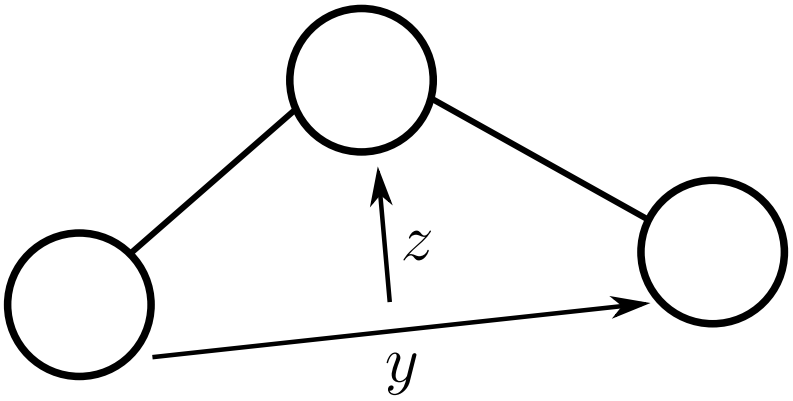


Figure 3.2: The coordinates y and z describe the internal degrees of freedom of the 3-bead chain.

$\{F, G\}_\psi$ is

$$\begin{aligned}
\{F,G\}_\psi &= -\left\langle \psi, \left(\frac{\delta F}{\delta m}\right)^{\#} \cdot \frac{\delta G}{\delta \psi} - \left(\frac{\delta G}{\delta m}\right)^{\#} \cdot \frac{\delta F}{\delta \psi} \right\rangle \\
&= -\int d^n x d^n y d^n z\, \psi \Bigg[\frac{\delta F}{\delta m_i} \frac{\partial}{\partial x^i}\left(\frac{\delta G}{\delta \psi}\right) + \frac{\partial}{\partial x^j}\left(\frac{\delta F}{\delta m_i}\right) y^j \frac{\partial}{\partial y^i}\left(\frac{\delta G}{\delta \psi}\right), \\
&\quad + \left(\frac{\partial^2}{\partial x^j \partial x^k}\left(\frac{\delta F}{\delta m_i}\right) y^j y^k + \frac{\partial}{\partial x^j}\left(\frac{\delta F}{\delta m_i}\right) z^j\right) \frac{\partial}{\partial z^i}\left(\frac{\delta G}{\delta \psi}\right) \\
&\quad - \frac{\delta G}{\delta m_i} \frac{\partial}{\partial x^i}\left(\frac{\delta F}{\delta \psi}\right) + \frac{\partial}{\partial x^j}\left(\frac{\delta G}{\delta m_i}\right) y^j \frac{\partial}{\partial y^i}\left(\frac{\delta F}{\delta \psi}\right) \\
&\quad - \left(\frac{\partial^2}{\partial x^j \partial x^k}\left(\frac{\delta G}{\delta m_i}\right) y^j y^k + \frac{\partial}{\partial x^j}\left(\frac{\delta G}{\delta m_i}\right) z^j\right) \frac{\partial}{\partial z^i}\left(\frac{\delta F}{\delta \psi}\right) \Bigg]. \qquad (3.4.1)
\end{aligned}$$

Let us consider Hamiltonians of the form $H = H_{fluids}[m, \rho] + H_s[\psi]$ where H_{fluids} is as in (2.6.11). The evolution of ρ and $u = \delta H/\delta m = m/\rho$ are the same as (3.2.15b, 3.2.15a), but the evolution equation for ψ and the body force $\mathcal{F}_i$ on the fluid become

$$\dot{\psi} = -\frac{\partial}{\partial x^i}\left(u^i \psi\right) - \frac{\partial}{\partial y^i}\left(\frac{\partial u^i}{\partial x^j} y^j \psi\right) - \frac{\partial}{\partial z^i}\left(\left[\frac{\partial^2 u^i}{\partial x^j \partial x^k} y^j y^k + \frac{\partial u^i}{\partial x^j} z^j\right] \psi\right), \qquad (3.4.2a)$$

$$\begin{aligned}
\mathcal{F}_i = \int d^n y d^n z\, \psi \Bigg[&- \frac{\partial}{\partial x^i}\left(\frac{\delta H_s}{\delta \psi}\right) + \frac{\partial}{\partial x^j}\left(y^j \frac{\partial}{\partial y^i}\left(\frac{\delta H_s}{\delta \psi}\right)\right) \\
&+ \frac{\partial}{\partial x^j}\left(z^j \frac{\partial}{\partial z^i}\left(\frac{\delta H_s}{\delta \psi}\right)\right) - \frac{\partial^2}{\partial x^j \partial x^k}\left(y^j y^k \frac{\partial}{\partial z^i}\left(\frac{\delta H_s}{\delta \psi}\right)\right) \Bigg]. \qquad (3.4.2b)
\end{aligned}$$

The term $(\partial^2 u^i/\partial x^j \partial x^k) y^j y^k$ in (3.4.2a) 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

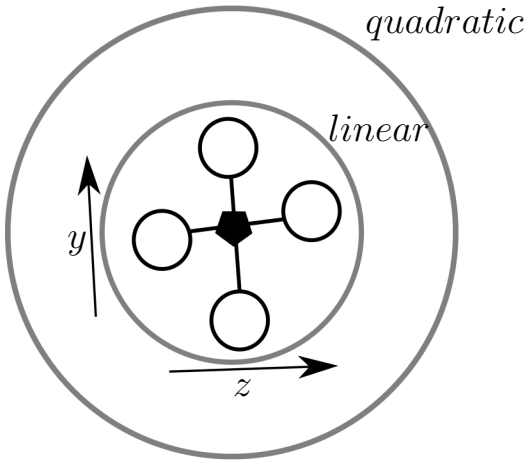


Figure 3.3: $(T \oplus T)M$ consists of a point on M, and a pair of tangent vectors y, z attached to that point. It is the configuration space of two bead-spring pairs with a common centre.

suspension couples to the second derivative of the flow velocity u, so it can detect *vorticity gradients* across the flow. As we shall demonstrate in section **3.4.2**, this model supports a force term $\mathcal{F}_i$ with nonzero torque, which means the stress tensor can be asymmetric [43, 45]. If we drop this term, the kinematics reduces to the conventional Rouse model [21], where the multibead-chains are affected by the local velocity gradient by not any higher derivatives.

In more geometrical terms, the flow vector field u would be acting on the configuration space $(T \oplus T)M$ instead of $T^{(2)}M$ if we ignore the second derivative term. Each point in $(T \oplus T)M$ consists of a pair of tangent vectors at a point on M. Figures 3.3 and 3.4 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 **A.2**. 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 **3.4.1**, 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 (3.4.2a), where $|y|$ is the lengthscale of the chain and $|x|$ is the gradient scale of the flow. One recovers the Rouse model by dropping this term.

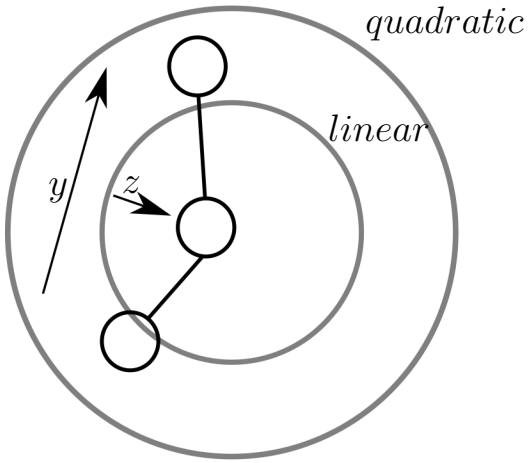


Figure 3.4: $T^{(2)}M$ consists of equivalence classes of paths $I \to M$ with the same Taylor series up to second order, with y, z being the first and second Taylor coefficients. It is the configuration space of a 3-bead chain.

3.4.1 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[2] g on $\mathbb{R}^{3n}$, which can be written as

$$ds^2 = \delta_{ij}dx^i dx^j + \delta_{ij}dy^i dy^j + \delta_{ij}dz^i dz^j. \tag{3.4.3}$$

We define the dissipation bracket

$$(F, G) = \int d^n x d^n y d^n z \; \psi \; \widetilde{g}\left(d\left(\frac{\delta F}{\delta \psi}\right), d\left(\frac{\delta G}{\delta \psi}\right)\right), \tag{3.4.4}$$

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

$$\begin{aligned}(F, G) = \int d^n x d^n y d^n z \; \psi \Bigg[& \delta^{ij} \frac{\partial}{\partial x^i}\left(\frac{\delta F}{\delta \psi}\right) \frac{\partial}{\partial x^j}\left(\frac{\delta F}{\delta \psi}\right) \\ & + \delta^{ij} \frac{\partial}{\partial y^i}\left(\frac{\delta F}{\delta \psi}\right) \frac{\partial}{\partial y^j}\left(\frac{\delta F}{\delta \psi}\right) + \delta^{ij} \frac{\partial}{\partial z^i}\left(\frac{\delta F}{\delta \psi}\right) \frac{\partial}{\partial z^j}\left(\frac{\delta F}{\delta \psi}\right) \Bigg].\end{aligned} \tag{3.4.5}$$

The dynamics is then given by

$$\frac{\partial F}{\partial t} = \{F, H\} - \frac{1}{\zeta}(F, H), \tag{3.4.6}$$

[2]The construction of Riemannian metrics on higher order tangent bundles of general Riemannian manifolds is considered in appendix **A.3**.

for some mobility parameter $1/\zeta$. Just like in the bead-spring pair model (section **3.2.4**), this dissipation bracket implements 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 (3.2.24), consider free energies of the form

$$H_s[\psi] = \int d^n x d^n y d^n z \ \left(E(y,z)\psi + k_B T \psi \log \psi\right), \tag{3.4.7}$$

with variational derivative $\delta H_s/\delta\psi = E(y,z) + k_B T\left(\log\psi + 1\right)$. The force can be written as the divergence of a stress tensor, $\mathcal{F}_i = \partial\sigma_i^j/\partial x^j$ in (3.4.2b), where

$$\begin{aligned}\sigma_i^j =& -3k_B T \int d^n y d^n z \ \psi + \int d^n y d^n z \ \psi \left(y^j \frac{\partial E}{\partial y^j} + z^j \frac{\partial E}{\partial z^j}\right) \\ &- \frac{\partial}{\partial x^k}\int d^n y d^n z \ \psi y^j y^k \frac{\partial E}{\partial z^k}.\end{aligned} \tag{3.4.8}$$

The evolution equation for ψ is obtained similarly:

$$\begin{aligned}&\frac{\partial\psi}{\partial t} + \frac{\partial}{\partial x^i}\left(u^i\psi\right) + \frac{\partial}{\partial y^i}\left(\frac{\partial u^i}{\partial x^j}y^j\psi\right) + \frac{\partial}{\partial z^i}\left(\left[\frac{\partial^2 u^i}{\partial x^j \partial x^k}y^j y^k + \frac{\partial u^i}{\partial x^j}z^j\right]\psi\right) \\ &\quad = \frac{1}{\zeta}\frac{\partial}{\partial y^i}\left(\delta^{ij}\frac{\partial E}{\partial y^j}\psi\right) + \frac{1}{\zeta}\frac{\partial}{\partial z^i}\left(\delta^{ij}\frac{\partial E}{\partial z^j}\psi\right) + \frac{k_B T}{\zeta}\left(\nabla_x^2\psi + \nabla_y^2\psi + \nabla_z^2\psi\right),\end{aligned} \tag{3.4.9}$$

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

$$E(y,z) = \frac{\kappa_1}{2}\delta_{ij}y^i y^j + \frac{\kappa_2}{2}\delta_{ij}z^i z^j. \tag{3.4.10}$$

By writing $\sigma^{jk} = \sigma_i^j \delta^{ik}$ and using the notation $\langle\cdots\rangle = \int d^n y d^n z \ \psi\left(\cdots\right)$, we can write the stress tensor (3.4.8) as

$$\sigma^{jk} = -3k_B T\left\langle 1\right\rangle \delta^{jk} + \kappa_1\left\langle y^j y^k\right\rangle + \kappa_2\left\langle z^j z^k\right\rangle - \kappa_2\frac{\partial}{\partial x^l}\left\langle y^j y^l z^k\right\rangle. \tag{3.4.11}$$

The evolution equation (3.4.9) for ψ then simplifies to

$$\begin{aligned}&\frac{\partial\psi}{\partial t} + \frac{\partial}{\partial x^i}\left(u^i\psi\right) + \frac{\partial}{\partial y^i}\left(\frac{\partial u^i}{\partial x^j}y^j\psi\right) + \frac{\partial}{\partial z^i}\left(\left[\frac{\partial^2 u^i}{\partial x^j \partial x^k}y^j y^k + \frac{\partial u^i}{\partial x^j}z^j\right]\psi\right) \\ &\quad = \frac{1}{\zeta}\frac{\partial}{\partial y^i}\left(y^i\psi\right) + \frac{1}{\zeta}\frac{\partial}{\partial z^i}\left(z^i\psi\right) + \frac{k_B T}{\zeta}\left(\nabla_x^2\psi + \nabla_y^2\psi + \nabla_z^2\psi\right).\end{aligned} \tag{3.4.12}$$

The stress tensor σ^{jk} in (3.4.11) 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* [43]. 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. In section **3.5**, we will discuss the interpretation of asymmetric stress tensors in generalised continuum systems.

The Hookean 3-bean chain model with dissipation terms conserves linear and angular momentum. This is consistent with *Noether's theorem*, since the energy $E(y, z)$ in (3.4.10) 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 (3.4.12) of ψ, we obtain the previous evolution equation (3.1.4) 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 (3.4.11) do not quite form a closed system, but this can be fixed by including a few extra moments.

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

In this section we show that the 3-bead chain model with quadratic energy (3.4.10), described by the equations (3.4.11, 3.4.12), has a finite and exact closure. We seek finite set of moments $\mu_1, \cdots, \mu_I$ of ψ, i.e. quantities of the form $\langle p(y, z) \rangle$ for polynomials p, such that the evolution of each moment can be expressed using this set of moments, together with u and its spatial derivatives:

$$\frac{\partial \mu_J}{\partial t} = f_J\left(\mu_1, \ldots, \mu_I; u\right) \quad \text{for } J = 1, \ldots, I, \tag{3.4.13}$$

and such that $\sigma = \sigma\left(\mu_1, \cdots, \mu_I; u\right)$ i.e. the stress tensor is completely described by these moments. To begin, since $\langle 1 \rangle, \left\langle y^j y^k \right\rangle, \left\langle z^j z^k \right\rangle, \left\langle y^i y^l z^k \right\rangle$ all appear in the expression for

σ^{jk}, let us look at their time derivatives:

$$\frac{\partial\langle 1\rangle}{\partial t}+\frac{\partial}{\partial x^i}\left(u^i\langle 1\rangle\right)=\frac{k_BT}{\zeta}\nabla_x^2\langle 1\rangle, \tag{3.4.14a}$$

$$\begin{aligned}\frac{\partial\langle y^jy^k\rangle}{\partial t}&+\frac{\partial}{\partial x^i}\left(u^i\langle y^jy^k\rangle\right)-\frac{\partial u^j}{\partial x^l}\langle y^ly^k\rangle-\frac{\partial u^k}{\partial x^l}\langle y^jy^l\rangle\\&=-\frac{2\kappa_1}{\zeta}\langle y^jy^k\rangle+\frac{2k_BT}{\zeta}\delta^{jk}\langle 1\rangle+\frac{k_BT}{\zeta}\nabla_x^2\langle y^jy^k\rangle,\end{aligned} \tag{3.4.14b}$$

$$\begin{aligned}\frac{\partial\langle z^jz^k\rangle}{\partial t}&+\frac{\partial}{\partial x^i}\left(u^i\langle z^jz^k\rangle\right)-\frac{\partial u^j}{\partial x^l}\langle z^lz^k\rangle-\frac{\partial u^k}{\partial x^l}\langle z^jz^l\rangle\\&-\frac{\partial^2u^j}{\partial x^m\partial x^l}\langle y^my^lz^k\rangle-\frac{\partial^2u^k}{\partial x^m\partial x^l}\langle y^my^lz^j\rangle\\&=-\frac{2\kappa_2}{\zeta}\langle z^jz^k\rangle+\frac{2k_BT}{\zeta}\delta^{jk}\langle 1\rangle+\frac{k_BT}{\zeta}\nabla_x^2\langle z^jz^k\rangle,\end{aligned} \tag{3.4.14c}$$

$$\begin{aligned}\frac{\partial\langle y^jy^lz^k\rangle}{\partial t}&+\frac{\partial}{\partial x^i}\left(u^i\langle y^jy^lz^k\rangle\right)-\frac{\partial u^j}{\partial x^m}\langle y^my^lz^k\rangle\\&-\frac{\partial u^l}{\partial x^m}\langle y^jy^mz^k\rangle-\frac{\partial u^k}{\partial x^m}\langle y^jy^lz^m\rangle-\frac{\partial^2u^k}{\partial x^m\partial x^n}\langle y^my^ny^jy^l\rangle\\&=-\frac{2\kappa_1}{\zeta}\langle y^jy^lz^k\rangle-\frac{\kappa_2}{\zeta}\langle y^jy^lz^k\rangle+\frac{2k_BT}{\zeta}\delta^{jl}\langle z^k\rangle+\frac{k_BT}{\zeta}\nabla_x^2\langle y^jy^lz^k\rangle.\end{aligned} \tag{3.4.14d}$$

The moments $\langle 1\rangle, \langle y^jy^k\rangle, \langle z^jz^k\rangle, \langle y^iy^lz^k\rangle$ do not quite form a closed system, as their time evolution depends on the extra moments $\langle y^my^ny^jy^l\rangle$ and $\langle z^k\rangle$. However, including the time evolution of just these extra moments closes the system:

$$\begin{aligned}&\frac{\partial\langle y^my^ny^jy^l\rangle}{\partial t}+\frac{\partial}{\partial x^i}\left(u^i\langle y^my^ny^jy^l\rangle\right)\\&\quad-\frac{\partial u^m}{\partial x^i}\langle y^iy^ny^jy^l\rangle-\frac{\partial u^n}{\partial x^i}\langle y^my^iy^jy^l\rangle-\frac{\partial u^j}{\partial x^i}\langle y^my^ny^iy^l\rangle-\frac{\partial u^l}{\partial x^i}\langle y^my^ny^jy^i\rangle\\&=-\frac{4\kappa_1}{\zeta}\langle y^my^ny^jy^l\rangle+\frac{k_BT}{\zeta}\nabla_x^2\langle y^my^ny^jy^l\rangle\\&\quad+\frac{2k_BT}{\zeta}\Big(\delta^{mn}\langle y^jy^l\rangle+\delta^{mj}\langle y^ny^l\rangle+\delta^{ml}\langle y^ny^j\rangle\\&\qquad+\delta^{nj}\langle y^my^l\rangle+\delta^{nl}\langle y^my^j\rangle+\delta^{jl}\langle y^my^n\rangle\Big),\end{aligned} \tag{3.4.14e}$$

$$\frac{\partial\langle z^k\rangle}{\partial t}+\frac{\partial}{\partial x^i}\left(u^i\langle z^k\rangle\right)-\frac{\partial u^k}{\partial x^i}\langle z^i\rangle-\frac{\partial^2u^k}{\partial x^m\partial x^n}\langle y^my^n\rangle=-\frac{\kappa_2}{\zeta}\langle z^k\rangle+\frac{k_BT}{\zeta}\nabla_x^2\langle z^k\rangle. \tag{3.4.14f}$$

So the moments $\langle 1\rangle, \langle y^jy^k\rangle, \langle z^jz^k\rangle, \langle y^iy^lz^k\rangle, \langle y^my^ny^jy^l\rangle, \langle z^k\rangle$ form a closed system of evolution equations. We can thus take these moments as the internal state variables of a macroscopic model for the Hookean 3-bead chain suspension[3].

[3]It is possible to interpret these moments as tensor fields – see appendix **A.2** 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 (3.4.11, 3.4.14a-f) as a *generalised continuum system* in section **3.5** and describe its behaviour under a shear flow in section **3.6**.

3.5 Generalised continuum systems

The study of *generalised continuum systems*, where the continuum possesses internal degrees of freedom that carry angular momentum, is initiated by the Cosserats [45]. The stress tensor is no longer required to be symmetric, and its antisymmetric part exchanges fluid angular momentum with internal angular momentum. This theory incorporates an additional term called the *couple stress*, which describes the surface torques between the internal degrees of freedom. Such systems are mainly constructed by postulating constitutive laws [97, 149, 167, 168], but there are also attempts to derive them from kinetic theory [46] or from homogenisation arguments [58, 63, 198]. The Hookean 3-bead chain model (3.4.11, 3.4.14a-f) is an example of a generalised continuum system derived from polymer kinetic theory.

The basic premise of generalised continuum systems comes from the conservation of linear momentum and total angular momentum, the latter of which includes contributions from both the fluid and the internal degrees of freedom. We will focus exclusively on fluids in a three-dimensional Euclidean domain $U \subset \mathbb{R}^3$ and forgo the distinction between upper (contravariant) and lower (covariant) indices in this section by identifying them using the standard Euclidean metric δ_{ij}. Consider a complex fluid suspension of objects with internal angular momentum. Following [43, 58, 149, 198], we write the momentum equation as

$$\rho \frac{Du_i}{Dt} = -\frac{\partial P}{\partial x_i} + \frac{\partial \sigma_{ki}}{\partial x_k} + \rho f_i, \tag{3.5.1}$$

where $D/Dt = \partial/\partial t + u_j \partial/\partial x_j$ is the material derivative, P is the pressure, σ_{ki} is the stress tensor, and f_i is any external body force per unit mass acting on the fluid. We keep the convention that the internal body force $\mathcal{F}_i$ is the divergence of the stress tensor against its *first* index – the other convention is also common in the literature. If we integrate (3.5.1) against a Lagrangian control volume V, we obtain

$$\begin{aligned} \frac{D}{Dt}\int_V dV\ \rho u_i &= -\int_V dV\ \frac{\partial P}{\partial x_i} + \int_V dV\ \frac{\partial \sigma_{ki}}{\partial x_k} + \int_V dV\ \rho f_i, \\ &= -\oint_{\partial V} dS\ n_i P + + \oint_{\partial V} dS\ n_k \sigma_{ki} + \int_V dV\ \rho f_i, \end{aligned} \tag{3.5.2}$$

where ∂V is the boundary of the control volume V and n_i is the outward unit normal of the control volume. This allows us to interpret $n_k\sigma_{ki}$ as a *surface force* acting on the control volume.

However, the effect of stress on the fluid angular momentum is not as straightforward. Taking the cross product with x_i of the momentum equation (3.5.1) and integrating against the same control volume V, we find (displaying pseudovectors as antisymmetric rank-2 tensors)

$$\begin{aligned}
&\frac{D}{Dt}\int_V dV\ \rho\left(x_i u_j - x_j u_i\right)\\
=&-\int_V dV\ \left(x_i\frac{\partial P}{\partial x_j} - x_j\frac{\partial P}{\partial x_i}\right) + \int_V dV\ \left(x_i\frac{\partial \sigma_{kj}}{\partial x_k} - x_j\frac{\partial \sigma_{ki}}{\partial x_k}\right)\\
&+\int_V dV\ \rho\left(x_i f_j - x_j f_i\right),\\
=&-\oint_{\partial V} dS\ \left(x_i n_j - x_j n_i\right)p + \oint_{\partial V} dS\ n_k\left(x_i\sigma_{kj} - x_j\sigma_{ki}\right)\\
&-\int_V dV\ \left(\sigma_{ij} - \sigma_{ji}\right) + \int_V dV\ \rho\left(x_i f_j - x_j f_i\right).
\end{aligned} \tag{3.5.3}$$

The term $\sigma_{ij} - \sigma_{ji}$ comes from the difference between

$$x_i\frac{\partial \sigma_{kj}}{\partial x_k} - x_j\frac{\partial \sigma_{ki}}{\partial x_k} \qquad \text{and} \qquad \frac{\partial}{\partial x_k}\left(x_i\sigma_{kj} - x_j\sigma_{ki}\right).$$

So the total torque due to the stress tensor comprises of a *surface torque*, which is the torque of the surface force $n_k\sigma_{ki}$, plus a *body torque* that is not the torque of any macroscopic force, which comes from the antisymmetric part of the stress tensor. The sink of fluid angular momentum $\sigma_{ij} - \sigma_{ji}$ due to an asymmetric stress tensor may appear to violate the conservation of angular momentum, but it can be considered as a source of *internal angular momentum* for a fluid with internal structure, so that the *total angular momentum* is still conserved.

Let M_{ij} be the total angular momentum density per unit mass. By considering torque balance on a Lagrangian control volume V, we have

$$\begin{aligned}
\frac{D}{Dt}\int_V dV\ \rho M_{ij} = &\int_V dV\ \rho\left(x_i f_j - x_j f_i + g_{ij}\right)\\
&-\oint_{\partial V} dS\ \left(x_i n_j - x_j n_i\right)p + \oint_{\partial V} dS\ n_k\left(c_{ikj} + x_i\sigma_{kj} - x_j\sigma_{ki}\right),
\end{aligned} \tag{3.5.4}$$

where g_{ij} is the external body torque on the internal degrees of freedom (such as any external magnetic field on a ferrofluid), and c_{ikj} is the *couple stress*, an angular momentum flux

arising from interactions of the internal degrees of freedom across the surface ∂V. The other terms are the torques of the macroscopic body force f_i and the macroscopic surface forces $-n_i p, n_k \sigma_{ki}$ on the fluid, respectively.

We define the *internal angular momentum density* l_{ij} to be the difference between the total angular momentum density and the fluid angular momentum density:

$$M_{ij} = x_i u_j - x_j u_i + l_{ij}. \tag{3.5.5}$$

Subtracting (3.5.3) from (3.5.4) gives an equation for l_{ij}

$$\frac{D}{Dt}\int_V dV\ \rho l_{ij} = \int_V dV\ \rho g_{ij} + \oint_{\partial V} dS\ n_k c_{ikj} + \int_V dV\ \left(\sigma_{ij} - \sigma_{ji}\right), \tag{3.5.6}$$

or in differential form,

$$\rho \frac{Dl_{ij}}{Dt} = \rho g_{ij} + \frac{\partial c_{ikj}}{\partial x_k} + \sigma_{ij} - \sigma_{ji}. \tag{3.5.7}$$

Combining equations (3.5.3, 3.5.7), we see that *the antisymmetric part of the stress tensor exchanges fluid angular momentum with internal angular momentum.*

The explicit expression for the couple stress c_{ikj}, much like the stress tensor σ_{ij}, has to be found from either a microscopic derivation or a constitutive relation. For the Hookean 3-bead chain model, the couple stress can be found from a torque balance argument. The antisymmetric part of the stress tensor in (3.4.11) is the divergence of a 3-index tensor:

$$\sigma_{ij} - \sigma_{ji} = -\kappa_2 \frac{\partial}{\partial x_k}\left(\langle y_i y_k z_j\rangle - \langle y_j y_k z_i\rangle\right). \tag{3.5.8}$$

Since the 3-bead chains are in a Stokes flow, they have no inertia, so the internal angular momentum density is identically zero. An instantaneous torque balance must then be maintained. In the absence of external torque on the internal degrees of freedom, the internal angular momentum equation (3.5.7) becomes

$$0 = \frac{\partial c_{ikj}}{\partial x_k} - \kappa_2 \frac{\partial}{\partial x_k}\left(\langle y_i y_k z_j\rangle - \langle y_j y_k z_i\rangle\right). \tag{3.5.9}$$

So (up to a curl) we can take the expression for the couple stress to be

$$c_{ikj} = \kappa_2\left(\langle y_i y_k z_j\rangle - \langle y_j y_k z_i\rangle\right). \tag{3.5.10}$$

Thus the instantaneous torque balance on the 3-bead chains create an extra angular momentum flux on the fluid, due to angular momentum being transmitted across a chain going through the bounding surface between adjacent fluid parcels. The appropriate boundary condition on walls is

$$n_k c_{ikj} = 0, \quad \text{where } n_k \text{ is the unit outward normal of the wall,} \tag{3.5.11}$$

since the chain cannot go through the wall.

3.6 The Hookean 3-bead chain suspension in a general shear flow

In this section we study the Hookean 3-bead chain model (3.4.11, 3.4.14a-f) in a general shear flow. We study two common benchmark problems in fluid dynamics, the first being the *Poiseuille flow* problem and the second being the *linearised (small Deborah number) Stokes problem*. We find that both problems exhibit a *couple stress boundary layer*. This is a typical feature of many generalised continuum systems [97, 149, 167, 168], where higher spatial derivatives are introduced in the equation due to the couple stress.

Again, we restrict our attention to fluids on a domain in three-dimensional Euclidean space $\mathbb{R}^3$. In this section only, we forgo the index notation in favour of the more explicit boldface dyadic notation for vectors and tensors. We denote the standard coordinates by (x_1, x_2, x_3) and the standard Euclidean basis by $\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3$. We also equip $\mathbb{R}^3$ with the standard dot product $\hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j = \delta_{ij}$.

Consider the evolution of the Hookean 3-bead chain system (3.4.14a–3.4.14e) under a general shear flow, where $\mathbf{u} = u(x_2, t)\hat{\mathbf{e}}_1$, and such that all quantities are functions of x_2 and time only. In particular, we have $\nabla \cdot \mathbf{u} = 0$ and $\mathbf{u} \cdot \nabla = 0$. To further simplify the set of equations, we ignore the diffusion terms $\nabla_x^2\langle \ldots \rangle$, as is customary in the rheological literature.

We rename the internal state tensors as

$$\mathbf{C} = \sum C_{ij}\hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j, \qquad C_{ij} = \langle y_i y_j \rangle, \tag{3.6.1a}$$

$$\mathbf{B} = \sum B_{ij}\hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j, \qquad B_{ij} = \langle z_i z_j \rangle, \tag{3.6.1b}$$

$$\mathbf{A} = \sum A_{ij}\hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j, \qquad A_{ij} = \langle y_i y_2 z_j \rangle, \tag{3.6.1c}$$

$$\mathbf{b} = \sum b_i\hat{\mathbf{e}}_i, \qquad b_i = \langle z_i \rangle, \tag{3.6.1d}$$

$$\chi_{ijkl} = \langle y_i y_j y_k y_l \rangle, \tag{3.6.1e}$$

$$n = \langle 1 \rangle. \tag{3.6.1f}$$

We assume the concentration n is constant, even though it is not strictly necessary in the following calculation for the steady-state stress tensor. The first and second velocity gradients can be written as

$$\frac{\partial \mathbf{u}}{\partial \mathbf{x}} = u'\hat{\mathbf{e}}_1 \otimes \hat{\mathbf{e}}_2, \qquad \frac{\partial^2 \mathbf{u}}{\partial \mathbf{x}\partial \mathbf{x}} = u''\hat{\mathbf{e}}_1 \otimes \hat{\mathbf{e}}_2 \otimes \hat{\mathbf{e}}_2. \tag{3.6.2}$$

For notational convenience, we define the purely geometric tensors

$$\mathbf{Q} = \hat{\mathbf{e}}_1 \otimes \hat{\mathbf{e}}_2, \qquad \mathbf{I} = \hat{\mathbf{e}}_1 \otimes \hat{\mathbf{e}}_1 + \hat{\mathbf{e}}_2 \otimes \hat{\mathbf{e}}_2 + \hat{\mathbf{e}}_3 \otimes \hat{\mathbf{e}}_3. \tag{3.6.3}$$

The particle-contributed stress (3.4.8) can then be written as

$$\boldsymbol{\sigma} = -3nk_BT\mathbf{I} + \kappa_1\mathbf{C} + \kappa_2\mathbf{B} - \kappa_2\frac{\partial}{\partial x_2}\mathbf{A}. \tag{3.6.4}$$

The only asymmetric term in the expression for the stress is the x_2-derivative of $A_{ij} = \langle y_i y_2 z_j \rangle$, because all moments are assumed to be functions of x_2 (and time). A relevant closed subset of the evolution equation is

$$\frac{\partial \mathbf{C}}{\partial t} - u'\mathbf{Q}\cdot\mathbf{C} - u'\mathbf{C}\cdot\mathbf{Q}^T = -\frac{2\kappa_1}{\zeta}\mathbf{C} + \frac{2nk_BT}{\zeta}\mathbf{I}, \tag{3.6.5a}$$

$$\frac{\partial \mathbf{B}}{\partial t} - u'\mathbf{Q}\cdot\mathbf{B} - u'\mathbf{B}\cdot\mathbf{Q}^T - u''\mathbf{Q}\cdot\mathbf{A} - u''\left(\mathbf{Q}\cdot\mathbf{A}\right)^T = -\frac{2\kappa_2}{\zeta}\mathbf{B} + \frac{2nk_BT}{\zeta}\mathbf{I}, \tag{3.6.5b}$$

$$\frac{\partial \mathbf{b}}{\partial t} - u'\mathbf{Q}\cdot\mathbf{b} - u''\hat{\mathbf{e}}_1 C_{22} = -\frac{\kappa_2}{\zeta}\mathbf{b}, \tag{3.6.5c}$$

$$\frac{\partial \mathbf{A}}{\partial t} - u'\mathbf{Q}\cdot\mathbf{A} - u'\mathbf{A}\cdot\mathbf{Q}^T - u''\begin{pmatrix}\chi_{2212}\\ \chi_{2222}\\ \chi_{2232}\end{pmatrix}\otimes\hat{\mathbf{e}}_1 = -\frac{2\kappa_1+\kappa_2}{\zeta}\mathbf{A} + \frac{2k_BT}{\zeta}\hat{\mathbf{e}}_2\otimes\mathbf{b}, \tag{3.6.5d}$$

$$\frac{\partial}{\partial t}\begin{pmatrix}\chi_{2212}\\ \chi_{2222}\\ \chi_{2232}\end{pmatrix} - u'\begin{pmatrix}\chi_{2222}\\ 0\\ 0\end{pmatrix} = -\frac{4\kappa_1}{\zeta}\begin{pmatrix}\chi_{2212}\\ \chi_{2222}\\ \chi_{2232}\end{pmatrix} + \frac{2k_BT}{\zeta}\begin{pmatrix}3C_{12}\\ 6C_{22}\\ 3C_{23}\end{pmatrix}. \tag{3.6.5e}$$

The last equation is obtained from taking the $2212, 2222, 2232$ components of (3.4.14e). Note that (3.6.5a) is precisely the equation for the conformation tensor in a shear flow in the upper-convected Maxwell model, up to some conventional factors[4] of 2.

3.6.1 Couple stress boundary condition on horizontal walls

In the following sections, we will often come across domains bounded by horizontal walls defined by $x_2 = const$. In addition to the usual no-slip boundary condition, there is also a no-internal angular momentum flux, or no-couple stress boundary condition on such walls.

The outward unit normal for a wall defined by by $x_2 = const$ is $\pm\hat{\mathbf{e}}_2$, where the sign depends on the orientation of the wall relative to the domain. Using (3.5.10, 3.5.11), the no-angular momentum flux boundary condition on such a wall is given by

$$c_{i2j} = \kappa_2\left(\langle y_i y_2 z_j\rangle - \langle y_j y_2 z_i\rangle\right) = 0, \tag{3.6.6}$$

[4]To recover the numerical factors that are common in the rheological literature, replace κ_1 with $2\kappa_1$ and $\mathbf{C}$ with $\mathbf{C}/2$. This replacement leaves the term $\kappa_1\mathbf{C}$ invariant, so it has no effect on the explicit expression of the stress tensor $\boldsymbol{\sigma}$. We keep to our current conventions with this in mind.

In terms of the internal state tensors we have defined in (3.6.1a–3.6.1e), this is equivalent to

$$\mathbf{A} - \mathbf{A}^T = 0 \quad \text{at walls with } x_2 = const. \tag{3.6.7}$$

This is the form of the no-couple stress boundary condition that will be particularly useful later.

3.6.2 Nondimensionalisation of the Hookean 3-bead chain equations

We proceed to nondimensionalise the system (3.6.5a-e). First we specify the *macroscopic scales* of the system. We denote nondimensionalised quantities with a tilde on top of the original dimensional quantity. Define the *system frequency scale* F, *system length scale* L and *system velocity scale* U, so that the independent variables x_2, t and the shear velocity u is nondimensionalised as follows:

$$\tilde{x}_2 = \frac{x_2}{L}, \quad \tilde{t} = Ft, \quad \tilde{u} = \frac{u}{U}. \tag{3.6.8}$$

The system frequency scale is not a priori related to the typical rate of shear U/L. This is important when the system is subject to some external time-dependent forcing. The choice of the scales F, L, U depends on the individual problem at hand.

We take the convention that the prime notation on dimensional quantities means $\partial/\partial x_2$ while the prime notation on dimensionless quantities means $\partial/\partial\tilde{x}_2$, for example $u' = \partial u/\partial x_2$, whereas $\tilde{u}' = \partial\tilde{u}/\partial\tilde{x}_2$.

Next, we nondimensionalise the internal state variables. Our choices are:

$$\tilde{\mathbf{C}} = \frac{\kappa_1}{nk_BT}\mathbf{C}, \tag{3.6.9a}$$

$$\tilde{\mathbf{B}} = \frac{\kappa_1}{nk_BT}\mathbf{B}, \tag{3.6.9b}$$

$$\tilde{\mathbf{A}} = \frac{\kappa_1}{nk_BT}L\frac{\kappa_1}{k_BT}\mathbf{A}, \tag{3.6.9c}$$

$$\tilde{\mathbf{b}} = \frac{\kappa_1}{nk_BT}L\mathbf{b}, \tag{3.6.9d}$$

$$\tilde{\chi} = \frac{\kappa_1}{nk_BT}\frac{\kappa_1}{k_BT}\chi. \tag{3.6.9e}$$

The resulting nondimensionalised equations (3.6.5a-e) have a number of dimensionless

parameters. They are:

$$\mathrm{St} = \frac{FL}{U}, \qquad \text{Strouhal number,} \tag{3.6.10a}$$

$$\mathrm{De} = \frac{\zeta}{2\kappa_1}\frac{U}{L}, \qquad \text{Deborah number,} \tag{3.6.10b}$$

$$s = \frac{\kappa_1}{\kappa_2}, \qquad \text{stiffness ratio,} \tag{3.6.10c}$$

$$\lambda^2 = \frac{k_B T}{\kappa_1 L^2}, \qquad \text{length ratio.} \tag{3.6.10d}$$

The Strouhal number St is the ratio of unsteady rates of change to the steady rate of shear; the Deborah number De is the ratio of the viscoelastic relaxation time to the shear timescale; the stiffness ratio s is the ratio between the stretching mode and the bending mode; the length ratio λ is the ratio of the thermal length of the chain to the macroscopic length.

Using this nondimensionalisation, the elastic stress (3.6.4) can be written as

$$\frac{\boldsymbol{\sigma}}{nk_BT} = -3\mathbf{I} + \tilde{\mathbf{C}} + \frac{1}{s}\tilde{\mathbf{B}} - \frac{\lambda^2}{s}\frac{\partial}{\partial \tilde{x}_2}\tilde{\mathbf{A}}, \tag{3.6.11}$$

and the evolution equations (3.6.5a-e) become

$$\mathrm{De}\left(\mathrm{St}\frac{\partial \tilde{\mathbf{C}}}{\partial \tilde{t}} - \tilde{u}'\mathbf{Q}\cdot\tilde{\mathbf{C}} - \tilde{u}'\tilde{\mathbf{C}}\cdot\mathbf{Q}^T\right) = -\tilde{\mathbf{C}} + \mathbf{I}, \tag{3.6.12a}$$

$$\mathrm{De}\left(\mathrm{St}\frac{\partial \tilde{\mathbf{B}}}{\partial \tilde{t}} - \tilde{u}'\mathbf{Q}\cdot\tilde{\mathbf{B}} - \tilde{u}'\tilde{\mathbf{B}}\cdot\mathbf{Q}^T - \lambda^2\tilde{u}''\left(\mathbf{Q}\cdot\tilde{\mathbf{A}} + \left(\mathbf{Q}\cdot\tilde{\mathbf{A}}\right)^T\right)\right) = -\frac{1}{s}\tilde{\mathbf{B}} + \mathbf{I}, \tag{3.6.12b}$$

$$\mathrm{De}\left(\mathrm{St}\frac{\partial \tilde{\mathbf{b}}}{\partial \tilde{t}} - \tilde{u}'\mathbf{Q}\cdot\tilde{\mathbf{b}} - \tilde{u}''\hat{\mathbf{e}}_1\tilde{C}_{22}\right) = -\frac{1}{2s}\tilde{\mathbf{b}}, \tag{3.6.12c}$$

$$\mathrm{De}\left(\mathrm{St}\frac{\partial \tilde{\mathbf{A}}}{\partial \tilde{t}} - \tilde{u}'\mathbf{Q}\cdot\tilde{\mathbf{A}} - \tilde{u}'\tilde{\mathbf{A}}\cdot\mathbf{Q}^T - u''\begin{pmatrix}\tilde{\chi}_{2212}\\ \tilde{\chi}_{2222}\\ \tilde{\chi}_{2232}\end{pmatrix}\otimes\hat{\mathbf{e}}_1\right) = -\frac{2s+1}{2s}\tilde{\mathbf{A}} + \hat{\mathbf{e}}_2\otimes\tilde{\mathbf{b}}, \tag{3.6.12d}$$

$$\mathrm{De}\left(\mathrm{St}\frac{\partial}{\partial \tilde{t}}\begin{pmatrix}\tilde{\chi}_{2212}\\ \tilde{\chi}_{2222}\\ \tilde{\chi}_{2232}\end{pmatrix} - \tilde{u}'\begin{pmatrix}\tilde{\chi}_{2222}\\ 0\\ 0\end{pmatrix}\right) = -2\begin{pmatrix}\tilde{\chi}_{2212}\\ \tilde{\chi}_{2222}\\ \tilde{\chi}_{2232}\end{pmatrix} + \begin{pmatrix}3\tilde{C}_{12}\\ 6\tilde{C}_{22}\\ 3\tilde{C}_{23}\end{pmatrix}. \tag{3.6.12e}$$

3.6.3 Discussion of asymptotic limits

To begin analysing the nondimensionalised system (3.6.12a-e), we investigate a few asymptotic limits in terms of the dimensionless parameters (3.6.10a-d). We restrict our attention to systems with Deborah numbers that are not too large $\mathrm{De} \lesssim O(1)$. The small Deborah number limit corresponds to an elastic response that decays quickly, which poses no mathematical or physical problems. However, if we formally take the large Deborah number limit, the leading order equation will be perfectly elastic while the relaxation terms only come in in the next order. While such systems exist physically, the perturbation theory of these weakly dissipative systems is much more mathematically involved, and for simplicity we avoid this scenario.

The evolution equation for the full distribution function of the bead chains is derived under the assumption that the bead chains are not too long, so that differences of the velocities of the individual beads are well-approximated by a Taylor series expansion of the background fluid velocity field $\mathbf{u}(x)$ about a fixed reference point on the chain. This is only valid when the bead chains are not too long compared to macroscopic lengthscales of the system. So the length ratio λ cannot be too large. A 3-point approximation to a chain is also problematic if the bending extension of the chain is too large compared to the stretching extension, which means the stiffness of the bending mode κ_2 should not be asymptotically small compared to the stiffness of the stretching mode κ_1. Thus the parameters λ^2 and s cannot be asymptotically large. We summarise our restrictions on the dimensionless parameters (3.6.10a-d) as follows:

$$\mathrm{De} \lesssim O(1), \qquad \lambda^2 \lesssim O(1), \qquad s \lesssim O(1). \tag{3.6.13}$$

We investigate the immediately accessible asymptotic limits $\lambda^2 \ll 1, s \sim O(1)$ and $\lambda^2 \sim O(1), s \ll 1$, assuming no particular ordering for De and St.

3.6.3.1 $\lambda^2 \ll 1, s \sim O(1)$

The limit $\lambda^2 \ll 1$ of having asymptotically short chains reduces the system (3.6.12a–3.6.12e) to something similar a generalised Maxwell model [20], or more precisely the moment equations for the Rouse model of a Hookean 3-bead chain [21, 51]. The asymmetric term in the expression for the elastic stress (3.6.11) vanishes in this limit. More explicitly,

$$\frac{\boldsymbol{\sigma}}{nk_BT} = -3\mathbf{I} + \tilde{\mathbf{C}} + \frac{1}{s}\tilde{\mathbf{B}} + O(\lambda^2). \tag{3.6.14}$$

The only relevant internal state tensors are $\tilde{\mathbf{C}}$ and $\tilde{\mathbf{B}}$, and they are both symmetric by construction. The relevant subset of evolution equations are

$$\mathrm{De}\left(\mathrm{St}\frac{\partial\tilde{\mathbf{C}}}{\partial\tilde{t}} - \tilde{u}'\mathbf{Q}\cdot\tilde{\mathbf{C}} - \tilde{u}'\tilde{\mathbf{C}}\cdot\mathbf{Q}^T\right) = -\tilde{\mathbf{C}} + \mathbf{I}, \tag{3.6.15a}$$

$$\mathrm{De}\left(\mathrm{St}\frac{\partial\tilde{\mathbf{B}}}{\partial\tilde{t}} - \tilde{u}'\mathbf{Q}\cdot\tilde{\mathbf{B}} - \tilde{u}'\tilde{\mathbf{B}}\cdot\mathbf{Q}^T\right) = -\frac{1}{s}\tilde{\mathbf{B}} + \mathbf{I} + O(\lambda^2). \tag{3.6.15b}$$

There are no longer terms depending on u'' at leading order. Thus the resulting stress can be decomposed into a pressure part $-\mathbf{I}$ and a pair of upper-convected Maxwell parts $\tilde{\mathbf{C}} - \mathbf{I}, (1/s)\tilde{\mathbf{B}} - \mathbf{I}$ with different relaxation times. We can thus recover the generalised upper-convected Maxwell model from the Hookean 3-bead chain model as a limit. The first non-vanishing order at which the asymmetric terms in the stress appears is $O(\lambda^2)$, which is typically much smaller than the symmetric part of the stress tensor.

3.6.3.2 $s \ll 1, \lambda^2 \sim O(1)$

Next we investigate the limit $s \ll 1$, where the bending stiffness is very large and the bending degree of freedom is essentially frozen. The stress now has a finite asymmetric part (still scaling as $\sim \lambda^2$) that can be determined from the evolution of the stretching mode only. The equations (3.6.12b, 3.6.12c, 3.6.12d) for $\tilde{\mathbf{B}}, \tilde{\mathbf{A}}, \tilde{\mathbf{b}}$ contains factors of $1/s$ in this limit, and so does the stress (3.6.11). This is not problematic since the first non-vanishing order of $\tilde{\mathbf{B}}, \tilde{\mathbf{A}}, \tilde{\mathbf{b}}$ are at $O(s)$.

Let us expand $\tilde{\mathbf{B}}, \tilde{\mathbf{A}}, \tilde{\mathbf{b}}$ in orders of s:

$$\begin{aligned}
\tilde{\mathbf{B}} &= \tilde{\mathbf{B}}^{(0)} + s\tilde{\mathbf{B}}^{(1)} + s^2\tilde{\mathbf{B}}^{(2)} + \dots, \\
\tilde{\mathbf{A}} &= \tilde{\mathbf{A}}^{(0)} + s\tilde{\mathbf{A}}^{(1)} + s^2\tilde{\mathbf{A}}^{(2)} + \dots, \\
\tilde{\mathbf{b}} &= \tilde{\mathbf{b}}^{(0)} + s\tilde{\mathbf{b}}^{(1)} + s^2\tilde{\mathbf{b}}^{(2)} + \dots,
\end{aligned}$$

and substitute these expansions into the respective evolution equations (3.6.12b, 3.6.12c, 3.6.12d). We also assume that the Strouhal number St is not asymptotically large, i.e. there is no asymptotically fast timescales that are comparable to $1/s$. The $O(1/s)$ balance of (3.6.12b, 3.6.12c, 3.6.12d) gives

$$\tilde{\mathbf{B}}^{(0)} = 0, \qquad \tilde{\mathbf{A}}^{(0)} = 0, \qquad \tilde{\mathbf{b}}^{(0)} = 0. \tag{3.6.16}$$

The $O(1)$ balance of (3.6.12b, 3.6.12c, 3.6.12d) then gives

$$0 = -\tilde{\mathbf{B}}^{(1)} + \mathbf{I}, \tag{3.6.17a}$$

$$-\mathrm{De}u'' \begin{pmatrix} \tilde{\chi}_{2212} \\ \tilde{\chi}_{2222} \\ \tilde{\chi}_{2232} \end{pmatrix} \otimes \hat{\mathbf{e}}_1 = -\frac{1}{2}\tilde{\mathbf{A}}^{(1)} \tag{3.6.17b}$$

$$-\mathrm{De}\tilde{u}''\hat{\mathbf{e}}_1\tilde{C}_{22} = -\frac{1}{2}\tilde{\mathbf{b}}^{(1)}. \tag{3.6.17c}$$

We can substitute this into the expression for the stress (3.6.11) to obtain

$$\frac{\boldsymbol{\sigma}}{nk_BT} = -2\mathbf{I} + \tilde{\mathbf{C}} - 2\mathrm{De}\lambda^2\frac{\partial}{\partial\tilde{x}_2}\left(\tilde{u}'' \begin{pmatrix} \tilde{\chi}_{2212} \\ \tilde{\chi}_{2222} \\ \tilde{\chi}_{2232} \end{pmatrix} \otimes \hat{\mathbf{e}}_1\right) + O(s), \tag{3.6.18}$$

where the time evolution of $\tilde{\mathbf{C}}$ and $\tilde{\chi}$ are governed by the remaining two equations (3.6.12a, 3.6.12e). Both $\tilde{\mathbf{C}}$ and $\tilde{\chi}$ are quantities that depend on the stretching degrees of freedom only. The finite asymmetric term in the stress tensor can be thought of as an angular momentum flux that comes from the instantaneous balance between the bending force exerted on the bead chains due to the curvature of the flow and the internal spring forces on the chain that resists bending.

3.6.4 Steady Poiseuille flow

Consider the flow problem for the 3-bead chain suspension in a channel bounded by walls $x_2 = 0$ and $x_2 = L$. Assuming $\mathbf{u} = u(x_2)\hat{\mathbf{e}}_1$ and that all quantities depend on x_2 only. The steady-state force balance is

$$\nabla\cdot\boldsymbol{\sigma} + \nabla\cdot\boldsymbol{\sigma}_N = -\rho\mathbf{f}, \tag{3.6.19}$$

where

$$\boldsymbol{\sigma}_N = \mu\begin{pmatrix} 0 & u' & 0 \\ u' & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{3.6.20}$$

is the Newtonian viscous stress, and

$$\mathbf{f} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \end{pmatrix} \tag{3.6.21}$$

is the external force per unit mass. The stress of the Hookean 3-bead chains $\boldsymbol{\sigma}$ in a steady state shear flow can be found from a simple but tedious calculation, which we relegate to appendix **B**.

The force balance equation is

$$\frac{\partial}{\partial x_2}\begin{pmatrix}\sigma_{21}\\ \sigma_{22}\\ \sigma_{23}\end{pmatrix}+\frac{\partial}{\partial x_2}\begin{pmatrix}\mu u'\\ 0\\ 0\end{pmatrix}=-\rho\begin{pmatrix}f_1\\ f_2\\ f_3\end{pmatrix}. \tag{3.6.22}$$

Assuming the concentration n is constant, the expression for $\boldsymbol{\sigma}$ derived in appendix **B** gives $\sigma_{22}=-nk_BT$ and $\sigma_{23}=0$. So the steady state does not support forces in the $\hat{\mathbf{e}}_2$ and $\hat{\mathbf{e}}_3$ directions. Restricting our attention to forces of the form $\mathbf{f}=f(x_2)\hat{\mathbf{e}}_1$ (so $f=f_1$), the force balance becomes

$$\frac{\partial}{\partial x_2}\sigma_{21}+\mu u''=-\rho f, \tag{3.6.23}$$

Given the dependence of the steady state shear stress σ_{21} on $u(x_2)$ (B.0.5c), this is an ordinary differential equation in $u(x_2)$. We will subsequently consider the Poiseuille flow problem, where f is constant.

We nondimensionalise the differential equation (3.6.23) as follows. We define the lengthscale L to be the width of the channel, and define the velocity scale U as

$$U=\frac{\rho f L^2}{\mu},\qquad \text{so that}\quad \frac{\mu U}{L^2}=\rho f. \tag{3.6.24}$$

We define a dimensionless *non-Newtonian parameter* ϵ to be the ratio of the elastic shear stress to the viscous shear stress:

$$\epsilon=\frac{nk_BT\mathrm{De}}{\mu U/L}=\frac{nk_BT\zeta}{2\kappa_1\mu}=\frac{\text{elastic shear stress}}{\text{viscous shear stress}}. \tag{3.6.25}$$

This is the reciprocal of the Ericksen number in the liquid crystals literature. In terms of this new dimensionless parameter ϵ, the force balance equation (3.6.23) is

$$\left(1+\epsilon(1+s)\right)\tilde{u}''-\epsilon\lambda^2\frac{2(3+2s)}{1+2s}\tilde{u}''''=-1. \tag{3.6.26}$$

The boundary conditions on the walls $\tilde{x}_2=0$ and $\tilde{x}_2=1$ are the no-slip and no-couple stress boundary conditions, as discussed in section **3.6.1**. This means $\tilde{u}=0$ and $\tilde{\mathbf{A}}-\tilde{\mathbf{A}}^T=0$ at the walls. Using the expression for $\tilde{\mathbf{A}}$ derived in appendix **B**, the second condition means $\tilde{A}_{21}=0$, which gives the condition $\tilde{u}''=0$. The Poiseuille flow problem can thus be formulated as the following boundary value problem:

$$\left(1+\epsilon(1+s)\right)\left(\tilde{u}''-\alpha^2\tilde{u}''''\right)=-1, \tag{3.6.27}$$

$$\tilde{u}(0)=\tilde{u}(1)=0,\qquad \tilde{u}''(0)=\tilde{u}''(1)=0, \tag{3.6.28}$$

where

$$\alpha = \lambda \sqrt{\frac{2\epsilon(3+2s)}{(1+\epsilon(1+s))\,(1+2s)}} \tag{3.6.29}$$

is the *(dimensionless) couple stress boundary layer width*. The fourth derivative term can be found in earlier works on couple stress systems [167, 168] using constitutive laws for the couple stress.

The solution to the nondimensionalised Poiseuille flow problem (3.6.27) with the no-slip and no-couple stress boundary conditions (3.6.28) is given explicitly as (dropping the subscript from $\tilde{x}_2$ for notational simplicity)

$$\tilde{u}(\tilde{x}) = \frac{1}{1+\epsilon(1+s)} \left(\frac{1}{2}\tilde{x}(1-\tilde{x}) + \alpha^2 \left(\frac{\cosh\left((\tilde{x}-1/2)/\alpha\right)}{\cosh\left(1/2\alpha\right)} - 1 \right) \right). \tag{3.6.30}$$

Figures 3.5 and 3.6 plots the solution $\tilde{u}(\tilde{x})$ for various values of α. The overall reduction in amplitude by a factor of $(1+\epsilon(1+s))^{-1}$ is due to the standard effect of *enhanced shear viscosity* in an upper-convected Maxwell model, and it does not change the geometric profile of the Poiseuille flow. We can account for this effect by changing the velocity scale to $U_* = U(1+\epsilon(1+s))^{-1}$.

More interesting is the effect of the parameter α. When α is small, the solution is a Newtonian Poiseuille flow plus a small perturbation. In the limit of $\alpha \to 0$, the solution has the following asymptotic form

$$\begin{aligned} \frac{1}{\alpha^2}\left(\frac{U}{U_*}\tilde{u}(\tilde{x}) - \frac{1}{2}\tilde{x}(1-\tilde{x}) \right) =& \frac{\cosh\left((\tilde{x}-1/2)/\alpha\right)}{\cosh\left(1/2\alpha\right)} - 1 \\ &\sim \exp\left(\frac{1}{\alpha}\left(\left| \tilde{x} - \frac{1}{2} \right| - \frac{1}{2} \right) \right) - 1. \end{aligned} \tag{3.6.31}$$

So there is a pair of exponentially decaying boundary layers of characteristic width α around $\tilde{x} = 0$ and $\tilde{x} = 1$. The Newtonian Poiseuille flow profile in the intermediate layer is shifted by $-\alpha^2$, proportional to the concentration of the suspended chains. Our solution coincides with the Poiseuille flows considered in [97, 167], where the additional couple stress term is assumed to be a function of the vorticity gradient in a constitutive relation.

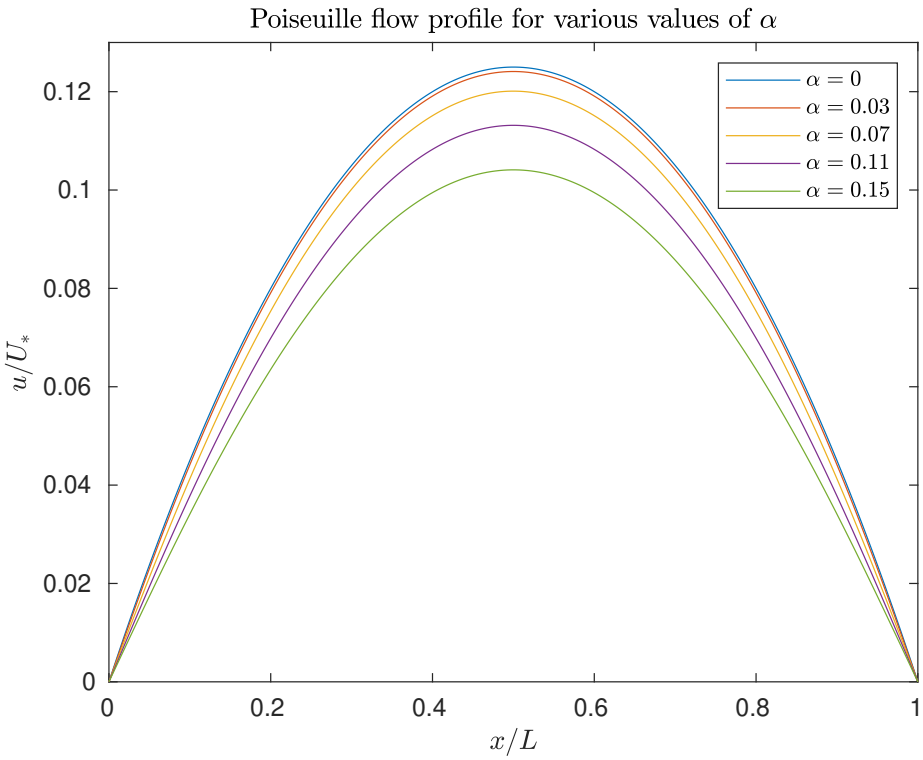


Figure 3.5: The Poiseuille flow profile for various values of α.

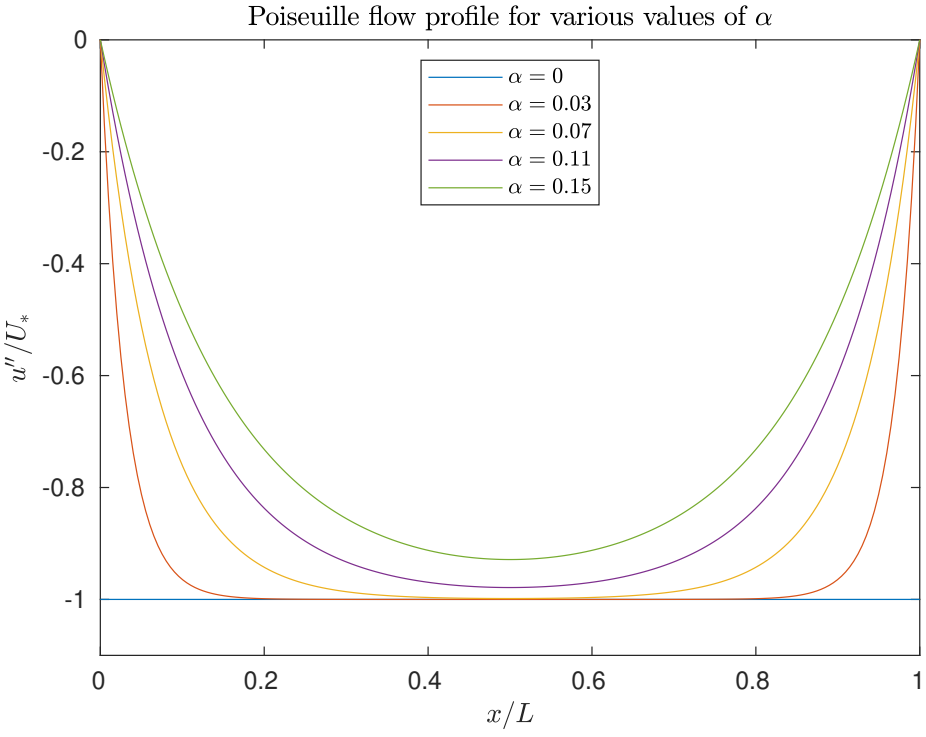


Figure 3.6: The second derivative of the Poiseuille flow profile for various values of α.

3.6.5 The linearised Stokes problem about a static equilibrium

In this section we consider the *Stokes problem* for the Hookean 3-bead chain suspension, linearised about a static equilibrium. The problem is formulated on a half-open domain $x_2 \geq 0$. At $t < 0$, the fluid in the half-open domain is at rest. For $t \geq 0$, a periodic perturbation of the bottom wall is introduced: $u(x_2 = 0, t) = U \sin(Ft)$, where we have chosen the sine so that $u(x_2, t)$ is continuous, and where U is small in an appropriate sense. We study the behaviour of the fluid in the domain for long times.

At $t < 0$, the fluid is at rest: $u(x_2, t < 0) = 0$. This is a particularly simple steady state. Substituting the zero flow steady state into the general solution for the (nondimensionalised) internal state tensors $\tilde{\mathbf{C}}, \tilde{\mathbf{B}}, \tilde{\mathbf{A}}, \tilde{\mathbf{b}}, \tilde{\chi}$ for any steady state shear flow in appendix **B** gives

$$\begin{gathered} \tilde{\mathbf{C}}(t<0) = \mathbf{I}, \quad \tilde{\mathbf{B}}(t<0) = s\mathbf{I}, \quad \tilde{\mathbf{A}}(t<0) = 0, \\ \tilde{\mathbf{b}}(t<0) = 0, \quad \tilde{\chi}_{2222}(t<0) = 3, \quad \tilde{\chi}_{2212}(t<0) = \tilde{\chi}_{2232}(t<0) = 0. \end{gathered} \tag{3.6.32}$$

We denote the deviation of these quantities from their steady state value with the prefix δ. For example, $\delta\tilde{\mathbf{C}} = \tilde{\mathbf{C}} - \tilde{\mathbf{C}}(t<0) = \tilde{\mathbf{C}} - \mathbf{I}$. We assume that these deviations are small, and linearise the evolution equations (3.6.12a-e) by dropping second order and higher terms in $\delta(\ldots)$.

Let us pause to consider the system scales and formulate the linearised equations in terms of a small dimensionless parameter. The velocity scale U and the frequency scale F are clearly set by the amplitude and the frequency of the vibrating bottom wall. What is less clear is the choice of a lengthscale L. Fortunately, the Stokes problem for a Newtonian fluid has a natural lengthscale associated to it, namely the *Stokes boundary layer width*

$$L = \sqrt{\frac{2\mu}{\rho F}}. \tag{3.6.33}$$

The choice of this lengthscale normalises the momentum equation for a shear flow in a Newtonian fluid (so $\epsilon = 0$) to the particularly simple form:

$$\frac{\partial \tilde{u}}{\partial \tilde{t}} = \frac{1}{2}\tilde{u}''. \tag{3.6.34}$$

The Stokes boundary layer width is the lengthscale at which the amplitude of the oscillation of $\tilde{u}$ decays away from the boundary. The only independent system scales are U and F with this choice, and we need to re-express the relevant dimensionless parameters (3.6.10a-d) in terms of U and F only:

$$\mathrm{StDe} = \frac{\zeta F}{2\kappa_1}, \qquad \mathrm{De} = \frac{\zeta U}{2\kappa_1}\sqrt{\frac{\rho F}{2\mu}}, \qquad \lambda^2 = \frac{k_B T}{\kappa_1}\frac{\rho F}{2\mu}. \tag{3.6.35}$$

The stiffness ratio s (3.6.10c) and the non-Newtonian parameter ϵ (3.6.25) are manifestly independent of U and F. The linearised Stokes equation can then be interpreted as an asymptotic limit where

$$\mathrm{De} \ll 1, \qquad \text{while } \mathrm{StDe} \sim O(1). \tag{3.6.36}$$

The Deborah number is small in this limit, but the combination StDe, which is the ratio of the viscoelastic relaxation timescale to the external driving timescale, is of order unity.

3.6.5.1 The linearised equations for the Stokes problem

In this subsection we find the linearised non-Newtonian stress and formulate the Stokes problem as a differential equation in the shear velocity $\tilde{u}$. To obtain an expression for the non-Newtonian stress, we proceed to linearise the evolution equations of the internal state tensors (3.6.12a-e) against the background (3.6.32). A relevant closed subset of the linearised equations is:

$$\mathrm{De}\left(\mathrm{St}\frac{\partial\delta\tilde{\mathbf{C}}}{\partial\tilde{t}} - \delta\tilde{u}'\left(\mathbf{Q}+\mathbf{Q}^T\right)\right) = -\delta\tilde{\mathbf{C}}, \tag{3.6.37a}$$

$$\mathrm{De}\left(\mathrm{St}\frac{\partial\delta\tilde{\mathbf{B}}}{\partial\tilde{t}} - s\delta\tilde{u}'\left(\mathbf{Q}+\mathbf{Q}^T\right)\right) = -\frac{1}{s}\delta\tilde{\mathbf{B}}, \tag{3.6.37b}$$

$$\mathrm{De}\left(\mathrm{St}\frac{\partial\delta\tilde{\mathbf{b}}}{\partial\tilde{t}} - \delta\tilde{u}''\hat{\mathbf{e}}_1\right) = -\frac{1}{2s}\delta\tilde{\mathbf{b}}, \tag{3.6.37c}$$

$$\mathrm{De}\left(\mathrm{St}\frac{\partial\delta\tilde{\mathbf{A}}}{\partial\tilde{t}} - 3\delta\tilde{u}''\hat{\mathbf{e}}_2\otimes\hat{\mathbf{e}}_1\right) = -\frac{2s+1}{2s}\delta\tilde{\mathbf{A}} + \hat{\mathbf{e}}_2\otimes\tilde{\mathbf{b}}. \tag{3.6.37d}$$

The equation for $\delta\tilde{\chi}$ is irrelevant to the form of the non-Newtonian stress – $\tilde{\chi}$ only enters through its steady state value.

The linearised evolution equations (3.6.37a-d) form a system of inhomogeneous linear first order ordinary differential equations in time, with the spatial variable $\tilde{x}_2$ entering only parametrically. Such systems are easily solved by the Laplace transform, which we define for functions $f(\tilde{t})$ of (nondimensionalised) time as[5]

$$\mathscr{L}[f](p) = \int_0^\infty \mathrm{d}\tilde{t}\mathrm{e}^{-p\tilde{t}}f(\tilde{t}). \tag{3.6.38}$$

[5]If the system has discontinuities at $\tilde{t}=0$, choosing the lower limit as 0^+ or 0^- results in slightly different dependence of the Laplace transforms of time derivatives on the initial conditions. Since our system is first order in time, and $\delta\tilde{u}, \delta\tilde{\mathbf{C}}, \delta\tilde{\mathbf{B}}, \delta\tilde{\mathbf{b}}, \delta\tilde{\mathbf{A}}$ are continuous at $\tilde{t}=0$, both conventions result in the same expressions.

The initial conditions for $\delta\tilde{u}, \delta\tilde{\mathbf{C}}, \delta\tilde{\mathbf{B}}, \delta\tilde{\mathbf{b}}, \delta\tilde{\mathbf{A}}$ are that they are all zero at $\tilde{t} = 0$. We denote the Laplace transform of a quantity with the same symbol of the quantity itself when no confusion can arise. The Laplace transform of (3.6.37a-d) is

$$\mathrm{StDe}p\delta\tilde{\mathbf{C}} - \mathrm{De}\delta\tilde{u}'\left(\mathbf{Q} + \mathbf{Q}^T\right) = -\delta\tilde{\mathbf{C}}, \tag{3.6.39a}$$

$$\mathrm{StDe}p\delta\tilde{\mathbf{B}} - s\mathrm{De}\delta\tilde{u}'\left(\mathbf{Q} + \mathbf{Q}^T\right) = -\frac{1}{s}\delta\tilde{\mathbf{B}}, \tag{3.6.39b}$$

$$\mathrm{StDe}p\delta\tilde{\mathbf{b}} - \mathrm{De}\delta\tilde{u}''\hat{\mathbf{e}}_1 = -\frac{1}{2s}\delta\tilde{\mathbf{b}}, \tag{3.6.39c}$$

$$\mathrm{StDe}p\delta\tilde{\mathbf{A}} - 3\mathrm{De}\delta\tilde{u}''\hat{\mathbf{e}}_2 \otimes \hat{\mathbf{e}}_1 = -\frac{2s+1}{2s}\delta\tilde{\mathbf{A}} + \hat{\mathbf{e}}_2 \otimes \delta\tilde{\mathbf{b}}. \tag{3.6.39d}$$

The solution is

$$\delta\tilde{\mathbf{C}} = \frac{\mathrm{De}\delta\tilde{u}'}{1 + \mathrm{StDe}p}\left(\mathbf{Q} + \mathbf{Q}^T\right), \tag{3.6.40a}$$

$$\delta\tilde{\mathbf{B}} = s\frac{s\mathrm{De}\delta\tilde{u}'}{1 + s\mathrm{StDe}p}\left(\mathbf{Q} + \mathbf{Q}^T\right), \tag{3.6.40b}$$

$$\delta\tilde{\mathbf{b}} = \frac{2s\mathrm{De}\delta\tilde{u}''}{1 + 2s\mathrm{StDe}p}\hat{\mathbf{e}}_1, \tag{3.6.40c}$$

$$\delta\tilde{\mathbf{A}} = s\frac{6\mathrm{De} + (4s\mathrm{De}/(1 + 2s\mathrm{StDe}p))}{(1 + 2s) + 2s\mathrm{StDe}p}\delta\tilde{u}''\hat{\mathbf{e}}_2 \otimes \hat{\mathbf{e}}_1. \tag{3.6.40d}$$

Substituting these expressions into the stress tensor (3.6.11) then gives

$$\begin{aligned}\frac{\delta\boldsymbol{\sigma}}{nk_BT} &= \delta\tilde{\mathbf{C}} + \frac{1}{s}\delta\tilde{\mathbf{B}} - \frac{\lambda^2}{s}\frac{\partial}{\partial\tilde{x}_2}\delta\tilde{\mathbf{A}} \\ &= \left(\frac{\mathrm{De}}{1 + \mathrm{StDe}p} + \frac{s\mathrm{De}}{1 + s\mathrm{StDe}p}\right)\left(\mathbf{Q} + \mathbf{Q}^T\right)\delta\tilde{u}' \\ &\quad - \lambda^2\frac{6\mathrm{De} + (4s\mathrm{De}/(1 + 2s\mathrm{StDe}p))}{(1 + 2s) + 2s\mathrm{StDe}p}\hat{\mathbf{e}}_2 \otimes \hat{\mathbf{e}}_1\delta\tilde{u}'''.\end{aligned} \tag{3.6.41}$$

The (dimensional) force on the fluid due to the non-Newtonian stress is $\partial\sigma_{21}/\partial x_2$. The Laplace transformed nondimensionalised fluid momentum equation is then

$$2p\delta\tilde{u} = \left(1 + \epsilon\left(\frac{1}{1 + \mathrm{StDe}p} + \frac{s}{1 + s\mathrm{StDe}p}\right)\right)\delta\tilde{u}'' - \lambda^2\epsilon\frac{6 + (4s/(1 + 2s\mathrm{StDe}p))}{(1 + 2s) + 2s\mathrm{StDe}p}\delta\tilde{u}''''. \tag{3.6.42}$$

3.6.5.2 Long-time behaviour of the linearised equations

We are interested in the long-time behaviour of the shear velocity in the Stokes problem (3.6.42). Since we have a boundary condition of the form

$$\tilde{u}(\tilde{x} = 0, \tilde{t}) = \mathrm{Im}\left(\exp\left(\mathrm{i}\tilde{t}\right)\right), \tag{3.6.43}$$

we expect that, after some initial transients, the flow will also have a response of a separable form $\tilde{u}(\tilde{x},\tilde{t}) \sim \mathrm{Im}\left(a(\tilde{x})\exp\left(\mathrm{i}\tilde{t}\right)\right)$. Employing an ansatz of this form is equivalent to only picking up the pole at $p = +\mathrm{i}$ in the inverse Laplace transform, discarding all transient data on the left half plane $\mathrm{Re}(p) < 0$. We thus only need to substitute $p = +\mathrm{i}$ in (3.6.42) to find this long-time response. This leads to an ordinary differential equation for the complex amplitude $a(\tilde{x})$[6] of the shear flow across the half-open domain:

$$2\mathrm{i}a = \left(1 + \epsilon\left(\frac{1}{1+\mathrm{i}\mathrm{StDe}} + \frac{s}{1+\mathrm{i}s\mathrm{StDe}}\right)\right)a'' - \lambda^2\epsilon\frac{6 + (4s/(1+2\mathrm{i}s\mathrm{StDe}))}{(1+2s)+2\mathrm{i}s\mathrm{StDe}}a''''. \tag{3.6.44}$$

The boundary conditions for $a(\tilde{x})$ are

$$\begin{aligned} a(\tilde{x}=0) = 1, \qquad & a''(\tilde{x}=0) = 0, \\ a(\tilde{x}), a'(\tilde{x}), a''(\tilde{x}), \ldots \to 0 \qquad & \text{as } \tilde{x} \to \infty. \end{aligned} \tag{3.6.45}$$

The first condition is the no-slip boundary condition at $\tilde{x} = 0$. The second condition is the no-couple stress boundary condition at $\tilde{x} = 0$, noting that the couple stress on the wall (3.6.7) is again proportional to u''. The third condition is a decay condition at infinity.

The differential equation (3.6.44) with the boundary conditions (3.6.45) has linearly independent solutions of the form $a(\tilde{x}) \propto \exp(\beta\tilde{x})$, for complex constants β that satisfy the following algebraic equation:

$$2\mathrm{i} = \left(1 + \epsilon\left(\frac{1}{1+\mathrm{i}\mathrm{StDe}} + \frac{s}{1+\mathrm{i}s\mathrm{StDe}}\right)\right)\beta^2 - \lambda^2\epsilon\frac{6 + (4s/(1+2\mathrm{i}s\mathrm{StDe}))}{(1+2s)+2\mathrm{i}s\mathrm{StDe}}\beta^4, \tag{3.6.46}$$

from which we obtain[7]

$$\beta_\pm^2 = \frac{\nu \pm \sqrt{\nu^2 - 8\mathrm{i}\eta}}{2\eta}, \tag{3.6.47a}$$

where

$$\nu = 1 + \epsilon\left(\frac{1}{1+\mathrm{i}\mathrm{StDe}} + \frac{s}{1+\mathrm{i}s\mathrm{StDe}}\right), \tag{3.6.47b}$$

$$\eta = \lambda^2\epsilon\frac{6 + (4s/(1+2\mathrm{i}s\mathrm{StDe}))}{(1+2s)+2\mathrm{i}s\mathrm{StDe}}. \tag{3.6.47c}$$

[6]For simplicity, we complexify the linear differential equation (3.6.42) and take the imaginary part after the relevant quantities are calculated.

[7]We place the branch cut of the complex square root on the negative real axis, so that $\mathrm{Re}\sqrt{z} > 0$ for all complex numbers z except when z is a non-positive real number.

Since $a(\tilde{x}) \propto \exp(\beta\tilde{x})$ tends to zero as $\tilde{x}$ tends to $+\infty$, the solutions for $\beta_\pm$ must have negative real part. This means

$$\beta_\pm = -\sqrt{\frac{\nu \pm \sqrt{\nu^2 - 8\mathrm{i}\eta}}{2\eta}}. \tag{3.6.48}$$

Using the boundary conditions (3.6.45), the solution to the differential equation (3.6.44) is

$$a(\tilde{x}) = \frac{\beta_-^2 \exp(\beta_+\tilde{x}) - \beta_+^2 \exp(\beta_-\tilde{x})}{\beta_-^2 - \beta_+^2}. \tag{3.6.49}$$

Figures 3.7 and 3.8 are plots of $a(\tilde{x})$ and $a''(\tilde{x})$ for some typical values of the parameters, compared to the case where the bending term is absent ($\lambda = 0$) and the purely Newtonian case ($\epsilon = 0$).

In the asymptotic limit $\eta \to 0$, which can be achieved by (say) taking the short chain limit $\lambda \to 0$, we have

$$\beta_+ \to -\sqrt{\frac{\nu}{\eta}} \qquad \sim O(\lambda^{-1}), \tag{3.6.50a}$$

$$\beta_- \to -\sqrt{\frac{2\mathrm{i}}{\nu}} \qquad \sim O(1), \tag{3.6.50b}$$

and the asymptotic solution for $a(\tilde{x})$ in this limit is

$$a(\tilde{x}) \sim \exp\left(-\sqrt{\frac{2\mathrm{i}}{\nu}}\tilde{x}\right) - \eta \exp\left(-\sqrt{\frac{\nu}{\eta}}\tilde{x}\right). \tag{3.6.51}$$

The first term is the ordinary Stokes boundary layer with a modified shear viscosity, as in a generalised upper-convected Maxwell model. The second term is a couple stress boundary layer term that decays on lengthscales of $O(\lambda)$, and has amplitude $O(\lambda^2)$. The same asymptotic analysis also applies in the dilute limit where the non-Newtonian parameter ϵ tends to zero, in which case the modified shear viscosity also tends to the usual Newtonian viscosity.

We are also interested in the behaviour of the solution to the linearised Stokes problem as we vary the concentration n of the 3-bead chains and the frequency F of the oscillation. From (3.6.25, 3.6.33, 3.6.35), the dependence of our parameters on n and F is

$$\epsilon \propto n, \quad \mathrm{StDe} \propto F, \quad \lambda^2 \propto F, \quad L \propto F^{-1/2}. \tag{3.6.52}$$

The non-Newtonian parameter ϵ is the only parameter that depends on the concentration n. The stiffness ratio s (3.6.10c) is independent of both n and F. Since we have linearised the problem for small U (or equivalently small De), our nondimensionalised solution does

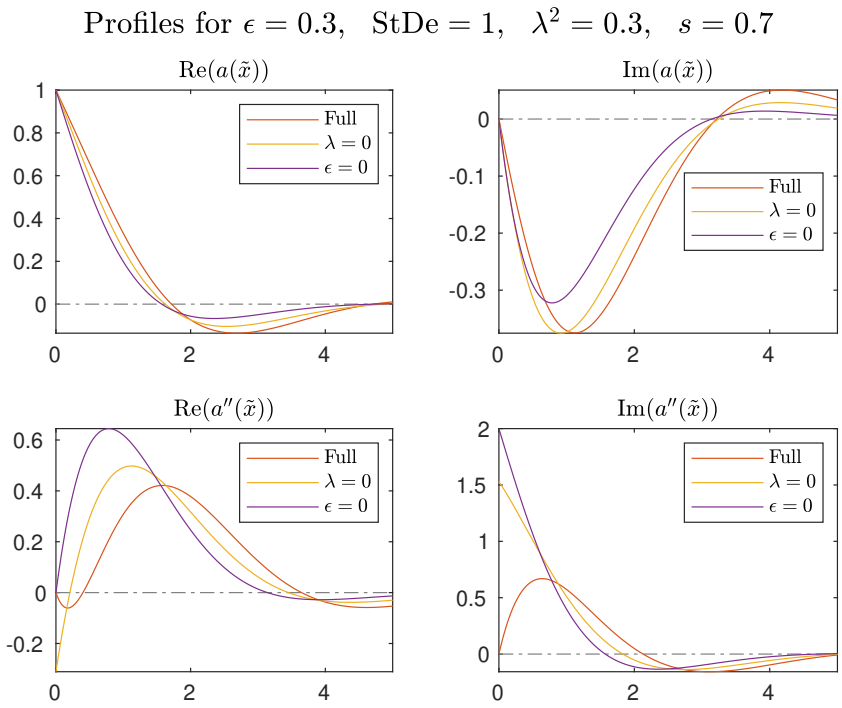


Figure 3.7: Plots of the real and imaginary parts of $a(\tilde{x})$.

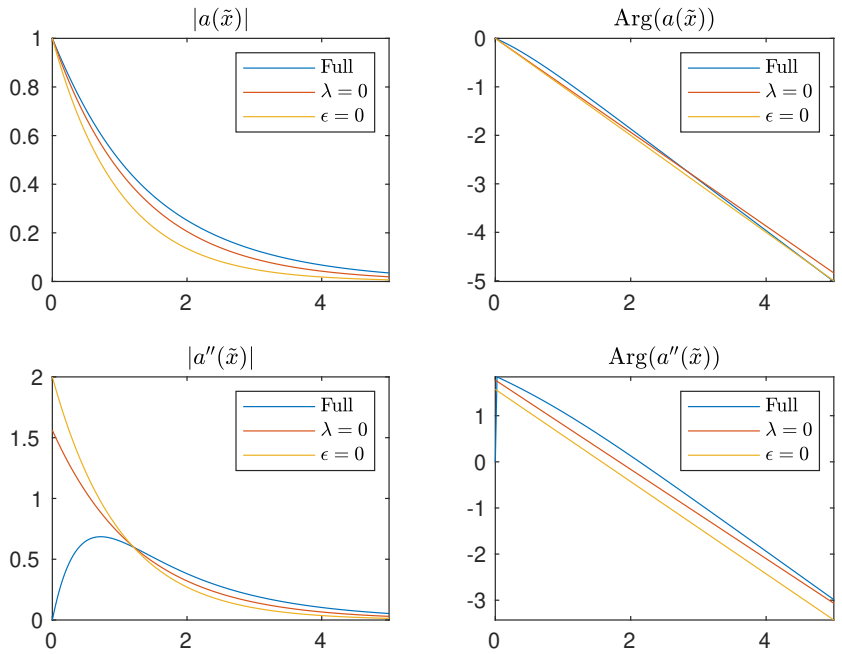


Figure 3.8: Plots of the magnitude and phase of $a(\tilde{x})$.

not depend on De. The main quantities of interest are $-\mathrm{Re}(\beta_\pm)$, as they are precisely the inverse widths of the exponentially decaying solution $a(\tilde{x})$, measured against the Stokes boundary layer width L. The imaginary parts $-\mathrm{Im}(\beta_\pm)$ are the spatial wavenumbers of the oscillations. Since the Stokes boundary layer width L also varies with frequency, we should also consider the quantities $\beta_\pm/L$ for the response of the observed decay widths and observed wavelengths to the changes in frequency. Figures 3.9 and 3.10 plot the variation of $\beta_\pm$ and $\beta_\pm/L$ with ϵ and F.

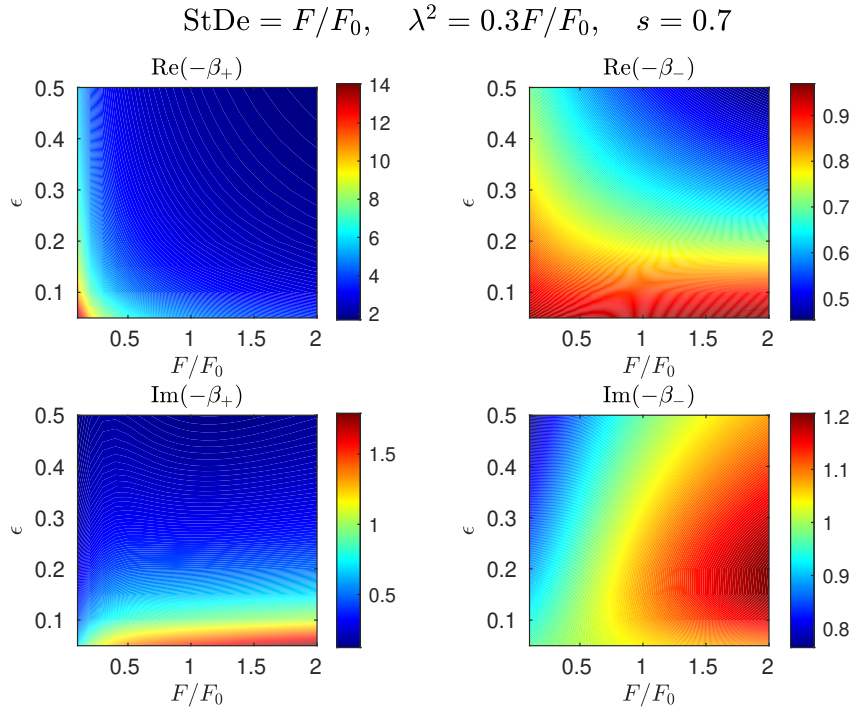


Figure 3.9: Plots of $\mathrm{Re}(\beta_\pm)$ and $\mathrm{Im}(\beta_\pm)$ for different values of ϵ and F.

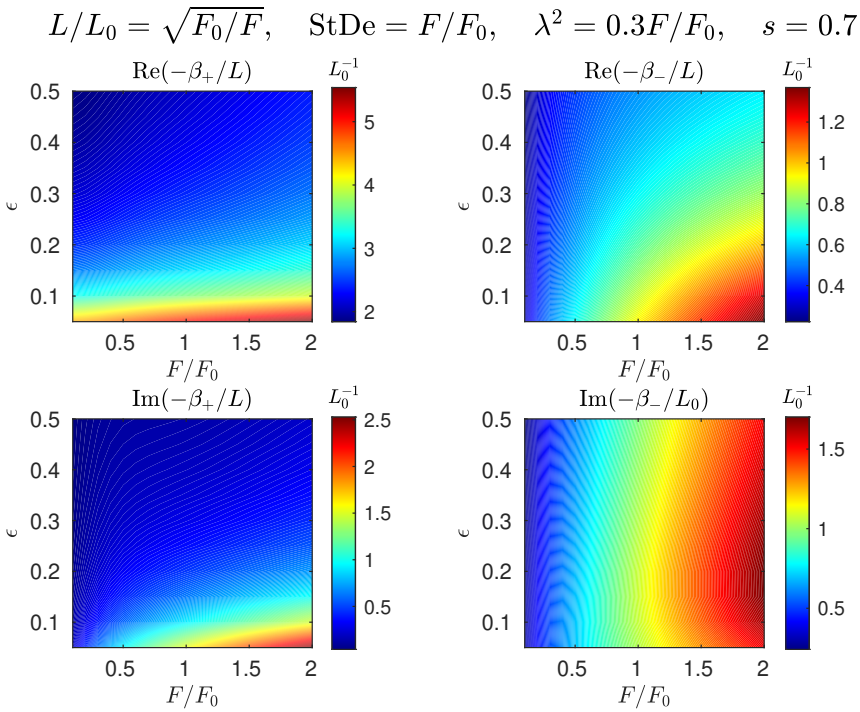


Figure 3.10: Plots of $\mathrm{Re}(\beta_\pm/L)$ and $\mathrm{Im}(\beta_\pm/L)$ for different values of ϵ and F.

3.7 The multibead-chain model

Having investigated the 3-bead chain in detail, we now return to the general case. In section **3.3** we have considered the action of vector fields $u \in \mathrm{Vect}(M)$ 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 semidirect product Lie–Poisson bracket (3.3.9).

We work exclusively in coordinates and take $M = \mathbb{R}^n$ in the following. Let x^i be coordinates on M and $(x^i, y^i_{(1)}, \ldots, y^i_{(N)})$ 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

$$d\Gamma = d^n y_{(1)} \cdots d^n y_{(N)}. \tag{3.7.1}$$

To write the components of the complete lift $u^{\#}$, defined in (3.3.6a, 3.3.6b) in terms of the components of $u(x)$ and its derivatives, we define the *exponential* of an operator X by the formal power series $\exp(X) = 1 + X + X^2/2! + \ldots$, and write

$$u^i(x+\delta x) = \exp\left(\delta x^j \frac{\partial}{\partial x^j}\right) u^i(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\delta x^j \frac{\partial}{\partial x^j}\right)^n u^i(x). \tag{3.7.2}$$

We only need a finite number of terms in the series in the following, so the convergence of the series is never an issue for later arguments. The components of $u^{\#}$ in the coordinate system $(x^i, y^i_{(1)}, \ldots, y^i_{(N)})$ can be written as $(u^i, u^i_{(1)} \ldots, u^i_{(N)})$, where

$$\begin{aligned} u^i_{(a)} &= \left(\frac{\partial}{\partial t}\right)^a \Big|_{t=0} u^i \left(x + \sum_{b=1}^{N} \frac{t^b}{b!} y_{(b)}\right), \\ &= \left(\frac{\partial}{\partial t}\right)^a \left[\exp\left(\sum_{b=1}^{N} \frac{t^b}{b!} y^j_{(b)} \frac{\partial}{\partial x^j}\right)\right]_{t=0} \cdot u^i(x), \\ &= \mathscr{P}_a\left(y_{(1)}, \ldots, y_{(N)}, \frac{\partial}{\partial x}\right) \cdot u^i(x). \end{aligned} \tag{3.7.3}$$

The expressions $\mathscr{P}_a$ are defined to be the a^{th} t-derivative of the exponential operator in the second line of (3.7.3). We can equivalently characterise $\mathscr{P}_a$ in terms of a generating function

$$\exp\left(\sum_{b=1}^{N} \frac{t^b}{b!} y^j_{(b)} \frac{\partial}{\partial x^j}\right) = 1 + \sum_{a=1}^{N} \frac{t^a}{a!} \mathscr{P}_a\left(y_{(1)}, \ldots, y_{(N)}, \frac{\partial}{\partial x}\right) + O(t^{N+1}). \tag{3.7.4}$$

Collecting powers of t in the exponential series shows that $\mathscr{P}_a$ is a polynomial in the *commuting* variables $y_{(1)}, \ldots, y_{(N)}, \partial/\partial x$. We write $\mathscr{P}_a = \mathscr{P}_a(y, \partial/\partial x)$ 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 $\mathscr{P}_a$ by collecting powers of t in (3.7.4):

(i) a is the highest power of $\partial/\partial x$ appearing $\mathscr{P}_a$.

(ii) 1 is the lowest power of $\partial/\partial x$ appearing $\mathscr{P}_a$. This means there is no "constant term" in $\mathscr{P}_a$ 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 $\mathscr{P}_a$ is a polynomial of order a in the variables $y_{(1)}, \dots, y_{(N)}$ with coefficients in $\partial/\partial x$. In particular, $\mathscr{P}_a$ 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 rewrite the term $\{F, G\}_\psi$ (3.3.10) in the Lie–Poisson bracket (3.3.9) as

$$\begin{aligned}
&\{F, G\}_\psi \\
&= -\int d^n x d\Gamma\ \psi \left[\frac{\delta F}{\delta m_i} \frac{\partial}{\partial x^i} \left(\frac{\delta G}{\delta \psi} \right) - \frac{\delta G}{\delta m_i} \frac{\partial}{\partial x^i} \left(\frac{\delta F}{\delta \psi} \right) \right] \\
&\quad - \int d^n x d\Gamma\ \psi \sum_{a=1}^{N} \left(\mathscr{P}_a \left(y, \frac{\partial}{\partial x} \right) \cdot \frac{\delta F}{\delta m_i} \right) \left(\frac{\partial}{\partial y^i_{(a)}} \frac{\delta G}{\delta \psi} \right) \\
&\quad + \int d^n x d\Gamma\ \psi \sum_{a=1}^{N} \left(\mathscr{P}_a \left(y, \frac{\partial}{\partial x} \right) \cdot \frac{\delta G}{\delta m_i} \right) \left(\frac{\partial}{\partial y^i_{(a)}} \frac{\delta F}{\delta \psi} \right), \\
&= \int d^n x d\Gamma\ \frac{\delta F}{\delta m_i} \left[-\psi \frac{\partial}{\partial x^i} \left(\frac{\delta G}{\delta \psi} \right) - \sum_{a=1}^{N} \mathscr{P}_a \left(y, -\frac{\partial}{\partial x} \right) \cdot \left(\psi \frac{\partial}{\partial y^i_{(a)}} \left(\frac{\delta G}{\delta \psi} \right) \right) \right] \\
&\quad + \int d^n x d\Gamma\ \frac{\delta F}{\delta \psi} \left[-\frac{\partial}{\partial x^i} \left(\frac{\delta G}{\delta m_i} \psi \right) - \sum_{a=1}^{N} \frac{\partial}{\partial y^i_{(a)}} \left(\left(\mathscr{P}_a \left(y, \frac{\partial}{\partial x} \right) \cdot \frac{\delta G}{\delta m_i} \right) \psi \right) \right].
\end{aligned} \tag{3.7.5}$$

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 $\mathscr{P}_a$ is a polynomial of degree a in $\partial/\partial x$. Given a Hamiltonian functional $H = H_{fluids}[m, \rho] + H_s[\psi]$, where H_{fluids} is as in (2.6.11), 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

$$\mathcal{F}_i = \int d\Gamma \left[-\psi \frac{\partial}{\partial x^i} \left(\frac{\delta H_s}{\delta \psi} \right) - \sum_{a=1}^{N} \mathscr{P}_a \left(y, -\frac{\partial}{\partial x} \right) \cdot \left(\psi \frac{\partial}{\partial y^i_{(a)}} \left(\frac{\delta H_s}{\delta \psi} \right) \right) \right], \tag{3.7.6a}$$

$$\dot{\psi} = -\frac{\partial}{\partial x^i} \left(u^i \psi \right) - \sum_{a=1}^{N} \frac{\partial}{\partial y^i_{(a)}} \left(\psi \mathscr{P}_a \left(y, \frac{\partial}{\partial x} \right) \cdot u^i \right), \tag{3.7.6b}$$

where $u^i = \delta H / \delta m_i = \delta^{ij} m_j / \rho$ as usual.

3.7.1 Conservation of fluid momentum for the multibead-chain models

We now specialise to Hamiltonians of the form

$$H[m, \rho, \psi] = H_{fluids}[m, \rho] + H_s[\psi], \quad H_s[\psi] = \int d^n x d\Gamma \left(E(y)\psi + k_B T \psi \log \psi \right), \tag{3.7.7}$$

where $E(y)$ is some function of the variables $y_{(1)}, \ldots, y_{(N)}$. The force on the fluid is given by (3.7.6a) as

$$\mathcal{F}_i = -(N+1) k_B T \frac{\partial}{\partial x^i} \left(\int d\Gamma \ \psi \right) - \int d\Gamma \ \sum_{a=1}^{N} \mathscr{P}_a \left(y, -\frac{\partial}{\partial x} \right) \cdot \left(\psi \frac{\partial E}{\partial y^i_{(a)}} \right). \tag{3.7.8}$$

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

$$\mathscr{P}_a \left(y, -\frac{\partial}{\partial x} \right) = \mathscr{Q}^j_a \left(y, -\frac{\partial}{\partial x} \right) \left(-\frac{\partial}{\partial x^j} \right) = -y^j_{(a)} \frac{\partial}{\partial x^j} + O\left(\frac{\partial^2}{\partial x^2} \right), \tag{3.7.9}$$

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

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

$$\sigma^j_i = -(N+1) k_B T \delta^j_i \int d\Gamma \ \psi + \int d\Gamma \ \sum_{a=1}^{N} \mathscr{Q}^j_a \left(y, -\frac{\partial}{\partial x} \right) \cdot \left(\psi \frac{\partial E}{\partial y^i_{(a)}} \right). \tag{3.7.10}$$

In particular, if $E(y)$ is a *polynomial* in $y_{(1)}, \cdots, y_{(N)}$, then σ^j_i 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 that $E(y)$ depends on the variables $y^i_{(a)}$ only through their Euclidean norms $s_{(a)} = (1/2)\delta_{ij}y^i_{(a)}y^j_{(a)}$, so that

$$E(y) = E\left(s_{(1)}, \ldots, s_{(N)}\right). \tag{3.7.11}$$

For $E(y)$ of the form (3.7.11), we have $\partial E/\partial y^i_{(a)} = \delta_{ik}y^k_{(a)}\partial E/\partial s_{(a)}$, so the stress tensor $\sigma^{jk} = \sigma^j_i\delta^{ik}$ can be written as

$$\sigma^{jk} = -(N+1)k_BT\delta^{jk}\left(\int d\Gamma\ \psi\right) + \sum_{a=1}^{N}\left(\int d\Gamma\ y^j_{(a)}y^k_{(a)}\frac{\partial E}{\partial s_{(a)}}\psi\right) + \frac{\partial}{\partial x^l}T^{jlk}, \tag{3.7.12}$$

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 **3.4.1**, as a term that is balanced by the divergence of a couple stress.

3.7.2 Closure of the multibead-chain models without dissipation

Having investigated the force term in (3.7.6a) and the relationship between the energy and the conservation laws in section **3.7.1**, we proceed to investigate the evolution equation (3.7.6b) for ψ in the multibead-chain model without dissipation. If $E(y)$ is a polynomial in $y_{(1)}, \cdots, y_{(N)}$, 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 $\mathscr{P}_a$ 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

$$\begin{aligned}\frac{\partial\langle p(y)\rangle}{\partial t} &= -\frac{\partial}{\partial x^i}\left(u^i(x)\left\langle p(y)\right\rangle\right) - \sum_{a=1}^{N}\int d\Gamma\ p(y)\frac{\partial}{\partial y^i_{(a)}}\left(\psi\mathscr{P}_a\left(y, \frac{\partial}{\partial x}\right)\cdot u^i(x)\right),\\ &= -\frac{\partial}{\partial x^i}\left(u^i(x)\left\langle p(y)\right\rangle\right) + \sum_{a=1}^{N}\left\langle\frac{\partial p(y)}{\partial y^i_{(a)}}\mathscr{P}_a\left(y, \frac{\partial}{\partial x}\right)\right\rangle\cdot u^i(x),\end{aligned} \tag{3.7.13}$$

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

Therefore

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

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 $y_{(1)}, \ldots, y_{(N)}$, 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.

3.7.3 The multibead-chain models with dissipation

Now we consider the multibead-chain model with a dissipation bracket. Consider the Riemannian metric[8] g on the configuration space of the multibead chain, with line element written as

$$ds^2 = \delta_{ij} dx^i dx^j + \sum_{a=1}^{N} \delta_{ij} dy^i_{(a)} dy^j_{(a)}, \tag{3.7.14}$$

and let $\widetilde{g}$ denote the inverse of g. We define a dissipation bracket on functionals F, G by

$$\begin{aligned}(F, G) &= \int d^n x d\Gamma \; \psi \widetilde{g} \left(d\left(\frac{\delta F}{\delta \psi} \right), d\left(\frac{\delta G}{\delta \psi} \right) \right), \\ &= \int d^n x d\Gamma \; \psi \left[\delta^{ij} \frac{\partial}{\partial x^i} \left(\frac{\delta F}{\delta \psi} \right) \frac{\partial}{\partial x^j} \left(\frac{\delta G}{\delta \psi} \right) + \sum_{a=1}^{N} \delta^{ij} \frac{\partial}{\partial y^i_{(a)}} \left(\frac{\delta F}{\delta \psi} \right) \frac{\partial}{\partial y^j_{(a)}} \left(\frac{\delta G}{\delta \psi} \right) \right].\end{aligned} \tag{3.7.15}$$

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

$$\frac{\partial F}{\partial t} = \{F, H\} - \frac{1}{\zeta}(F, H) \tag{3.7.16}$$

[8] See appendix **A.3** for a discussion for generalisations to arbitrary Riemannian manifolds.

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 is modified in a way that affects the closure properties of the system.

Consider free energies of the form (3.7.7), and further specialise to energy functions $E(y)$ that are *quadratic* in each internal degree of freedom, i.e.

$$E(y) = \sum_{a=1}^{N} \frac{\kappa_a}{2} \delta_{ij} y^i_{(a)} y^j_{(a)}, \tag{3.7.17}$$

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 **3.7.2**. The evolution equation for ψ is then

$$\begin{aligned} &\frac{\partial \psi}{\partial t} + \frac{\partial}{\partial x^i}\left(u^i(x)\psi\right) + \sum_{a=1}^{N} \frac{\partial}{\partial y^i_{(a)}} \left(\psi \mathscr{P}_a \left(y, \frac{\partial}{\partial x} \right) \cdot u^i(x) \right) \\ &\qquad = \frac{k_B T}{\zeta} \nabla^2_x \psi + \sum_{a=1}^{N} \left(\frac{\kappa_a}{\zeta} \frac{\partial}{\partial y^i_{(a)}} \left(y^i_{(a)} \psi \right) + \frac{k_B T}{\zeta} \nabla^2_{y_{(a)}} \psi \right), \end{aligned} \tag{3.7.18}$$

where $\nabla^2_x = \delta^{ij} \partial^2 / \partial x^i \partial x^j$, and $\nabla^2_{y_{(a)}} = \delta^{ij} \partial^2 / \partial y^i_{(a)} \partial y^j_{(a)}$ for $a = 1, \ldots, N$. 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 (3.7.10, 3.7.12):

$$\begin{aligned} \sigma^{jk} &= -(N+1) k_B T \delta^{jk} \int d\Gamma \; \psi + \sum_{a=1}^{N} \int d\Gamma \; \kappa_a y^k_{(a)} \mathscr{Q}^j_a \left(y, -\frac{\partial}{\partial x} \right) \cdot \psi, \\ &= -(N+1) k_B T \delta^{jk} \int d\Gamma \; \psi \\ &\qquad + \sum_{a=1}^{N} \int d\Gamma \; \kappa_a y^j_{(a)} y^k_{(a)} \psi + \frac{\partial}{\partial x^l} \left(\sum_{a=1}^{N} \int d\Gamma \; y^k_{(a)} \mathscr{R}^{jl}_a \left(y, -\frac{\partial}{\partial x} \right) \cdot \psi \right), \end{aligned} \tag{3.7.19}$$

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

$$\mathcal{P}_a\left(y,-\frac{\partial}{\partial x}\right)=\mathcal{Q}_a^j\left(y,-\frac{\partial}{\partial x}\right)\left(-\frac{\partial}{\partial x^j}\right)=-y^j_{(a)}\frac{\partial}{\partial x^j}+\mathcal{R}_a^{jl}\left(y,-\frac{\partial}{\partial x}\right)\frac{\partial^2}{\partial x^j\partial x^l}. \tag{3.7.20}$$

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 (3.7.19) does not exceed $2N$.

The hydrodynamic terms, the drift terms and the x-diffusion term in the evolution equation (3.7.18) 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 **3.4.2**, where the monomial moments required are precisely those of orders 0,2 and 4.

An apparently more general sufficient condition on $E(y)$ for a finite closure to be possible is that

$$\text{for all } a=1,\dots,N,\ \frac{\partial E}{\partial y^j_{(a)}} \text{ is a polynomial in } y \text{ of order less than or equal to } a. \tag{3.7.21}$$

This property is evidently satisfied for quadratic energies. We call a polynomial $p(y)$ satisfying property (3.7.21) *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

$$\frac{1}{\zeta}\sum_{a=1}^{N}\frac{\partial}{\partial y^i_{(a)}}\left(\delta^{ij}\frac{\partial E}{\partial y^j_{(a)}}\psi\right).$$

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 or 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 (3.7.17).

While $E(y)$ being admissible is nominally more general than $E(y)$ being of the Hookean-like form (3.7.17), we have the following highly constraining result:

Proposition 3.1. *$E(y)$ is admissible (in the sense of (3.7.21)) if and only if*

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

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

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

Then

$$\frac{\partial}{\partial y^j_{(a)}} (pq) = \frac{\partial p}{\partial y^j_{(a)}} q + p \frac{\partial q}{\partial y^j_{(a)}}$$

has order strictly greater than a, since q is not identically zero, and $\partial p / \partial y^j_{(a)}$ 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 $p(y) = \tau_{ij} y^i_{(a)} y^j_{(b)}$ 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

$$\frac{\partial}{\partial y^k_{(a)}} \left(\tau_{ij} y^i_{(a)} y^j_{(b)} \right) = \tau_{kj} y^j_{(b)} \text{ has order } b > a,$$

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

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

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

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

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. □

In particular, among all the admissible (in the sense of (3.7.21)) choices of energy functions $E(y)$, only the Hookean-like energy functions considered in (3.7.17) 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 [21, 148].

3.8 Conclusion

The main focus of this chapter 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 $\psi(x, y, t)$ 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 semidirect product Lie–Poisson bracket. 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 $\psi(x, y, t)$.

One of the main advantages for such a double bracket formulation is that, given a Hamiltonian functional that can be written in the form $H = H_{fluids}[m, \rho] + H_s[\psi]$, 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 known as the couple stress tensor in the theory of generalised continuum systems [43, 45, 58, 149, 198]. 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. We find that the asymmetric term leads to couple stress boundary layers in a shear flow, which is a ubiquitous feature in many generalised continuum systems [97, 149, 167, 168].

A major concern in using a kinetic model for the multibead-chains is that the evolution equation of $\psi(x, y, t)$ 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 $\psi(x, y, t)$. 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 u 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 a multibead-chain suspension. These new models can be considered as generalisations of the upper-convected Maxwell model for bead-spring pairs.

Within the framework of the kinetic model, 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 $\psi(x, y, t)$, 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 is the macroscopic model, which resolves this problem of dimensionality. Such models assumes that a set of internal state variables, which are phenomenological x-dependent fields, completely characterise the internal structure of the complex fluids. The macroscopic fluid properties such as the particle-contributed stress are then postulated to be completely determined by the chosen internal state variables through some constitutive equation. 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 (see section **2.3.2**). The conservative part is again captured by a semidirect product Lie–Poisson bracket. Examples of such complex fluid systems can be found in [16, 17, 57, 78, 79, 119].

However, the macroscopic description has a different problem – the equations are comparatively 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. In particular, 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 for 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 kinetic model, 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 $\psi(x, y, t)$, 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 $\psi(x, y, t)$ [78]. 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 $\psi(x, y, t)$. The governing equations are completely determined by the internal microphysics of the suspended bodies without any additional arbitrary modelling assumptions. When an exact closure is possible, the kinetic model reduces to the macroscopic model – such reduction also selects the appropriate internal state variables that are necessary for a complete macroscopic description of the suspension.

We believe that kinetic models and macroscopic models for complex fluids are very much interconnected, and the approaches inform each other. We suggest a *combined approach* for

modelling complex fluids, where the kinetic model is used as a starting point to implement the microphysics of the complex fluid. We can then make approximations to obtain effective equations for a set of internal state variables, leading to an approximate closure of the kinetic model to a macroscopic model. This approach is already applied in bead-spring pair suspensions [21, 148], and we hope that this chapter will inspire future work in the interplay between kinetic and macroscopic models for more complicated systems such as multibead-chain suspensions.

Chapter 4

Poisson maps from kinetic theory to hydrodynamics

In this chapter, we consider the kinetic theory of dilute monatomic gases and electrostatic plasmas. We study the various Hamiltonian reductions from kinetic theory to hydrodynamics in each system. This chapter is based on the author's work in [42]. Sections **4.1** and **4.2** reviews background material on Hamiltonian reductions in gas kinetic theory [71, 72, 74, 103, 126, 129, 130, 143, 172, 176, 189]. Sections **4.3** and **4.4** present the author's new results in the Hamiltonian reduction of kinetic theory to hydrodynamics [42]. Section **4.5** reviews hydrodynamic reductions of kinetic theory from singular Poisson submanifolds [39, 70, 72, 73, 144, 176, 177, 195]. We indicate some possible extensions of the considerations in this chapter to galactic dynamics and quantum mechanics in section **4.6**.

4.1 Introduction – Hamiltonian hierarchy of kinetic dilute gas models

There is a hierarchy of descriptions for the dynamics of a dilute monatomic gas in classical mechanics. These models are noncanonical Hamiltonian systems and they are often related by exact or approximate Hamiltonian reduction (see section **2.5**). In the following we introduce these models along the hierarchy, and explain the connection between them [103, 126, 143]. For simplicity we assume that the domain of the gas is $\mathbb{R}^3$ – the discussion generalises to Riemannian manifolds M without difficulty.

The first model is the full *N-body description*. The state of the gas is described by a point $z = (x_1, p_1, \ldots, x_N, p_N)$ in the full phase space $\mathbb{R}^{6N}$, where x_a and p_a are the position

and momentum of particle a. The time evolution is given by Hamilton's equations

$$\frac{dx_a}{dt} = \{x_a, H_N\}\,, \tag{4.1.1a}$$

$$\frac{dp_a}{dt} = \{p_a, H_N\}\,, \tag{4.1.1b}$$

for $a = 1, \dots N$, where $H_N(x_1, p_1, \dots, x_N, p_N)$ is the N-particle Hamiltonian and $\{\cdot, \cdot\}$ is the canonical Poisson bracket on $\mathbb{R}^{6N}$:

$$\{f, g\} = \sum_{a=1}^{N} \frac{\partial f}{\partial (x_a)^i} \frac{\partial g}{\partial (p_a)_i} - \frac{\partial g}{\partial (x_a)^i} \frac{\partial f}{\partial (p_a)_i}, \tag{4.1.2}$$

for functions $f, g \in C^\infty(\mathbb{R}^{6N})$. Equations (4.1.1a,b) is a canonical Hamiltonian system on the symplectic manifold $\mathbb{R}^{6N}$.

Averaging over an ensemble of initial conditions leads to the *N-particle kinetic description*, where the joint probability distribution function $\rho_N(x_1, p_1, \dots, x_N, p_N, t)$ for the positions and momenta of all N particles evolves according to the *Liouville equation*

$$\frac{\partial \rho_N}{\partial t} + \{\rho_N, H_N\} = 0, \tag{4.1.3}$$

where $\{\cdot, \cdot\}$ is the canonical Poisson bracket on $\mathbb{R}^{6N}$. Equation (4.1.1b) is a noncanonical Hamiltonian system on the Poisson manifold $C^\infty(\mathbb{R}^{6N})$ (see section **2.3.4**), with Hamiltonian functional

$$H[\rho_N] = \int dV_{6N}\; H_N(x_1, p_1, \dots, x_N, p_N)\rho_N, \tag{4.1.4}$$

where dV_{6N} is the standard symplectic volume form on $\mathbb{R}^{6N}$. The N-body description and the N-particle kinetic descriptions are related by a "singular moment map"

$$\begin{aligned}(\tilde{x}_1, \tilde{p}_1, \dots, \tilde{x}_N, \tilde{p}_N) \mapsto &\rho(x_1, p_1, \dots, x_N, p_N) \\ &= \delta^3(x_1 - \tilde{x}_1)\delta^3(p_1 - \tilde{p}_1) \dots \delta^3(x_N - \tilde{x}_N)\delta^3(p_N - \tilde{p}_N),\end{aligned} \tag{4.1.5}$$

whose image is a distribution rather than a smooth function on $\mathbb{R}^{6N}$. Many nonlinear functionals stop making sense for such ρ_N in (4.1.5), but each linear functional $\int dV_{6N}\; \rho_N g$ for $g \in C^\infty(\mathbb{R}^{6N})$ pulls back to g itself and generates the Hamiltonian flow of g on $\mathbb{R}^{6N}$ [70, 177].

If the N-particle Hamiltonian H_N is invariant under the action of permutations σ on the particles by $(x_a, p_a) \mapsto (x_{\sigma(a)}, p_{\sigma(a)})$, then the joint probability distribution function $\rho_N(x_1, p_1, \dots, x_N, p_N, t)$ will also be invariant under such permutations at all times if it is initially invariant. We denote this subspace of permutation-invariant distribution functions by $C^\infty_{sym}(\mathbb{R}^{6N})$ and restrict the noncanonical Hamiltonian system (4.1.3) to $C^\infty_{sym}(\mathbb{R}^{6N})$.

Let us further restrict our attention to gas particles that interact only through a pairwise potential $\phi(|q_a - q_b|)$, where $1 \leq a < b \leq N$, so that the N-particle Hamiltonian becomes

$$H_N(x_1, p_1, \ldots, x_N, p_N) = \sum_{a=1}^{N} \frac{|p_a|^2}{2} + \sum_{1 \leq a < b \leq N} \phi(|x_a - x_b|), \tag{4.1.6}$$

where we have assumed the particles have unit mass. The Liouville equation (4.1.3) then transforms into the Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) hierarchy [23, 31, 37, 64, 103, 126]. The dynamical variables in the BBGKY hierarchy are the *s-particle distribution functions* $f_s(x_1, p_1, \ldots, x_s, p_s, t)$, each of which gives the expected number of s-tuples of particles with prescribed positions and momenta. The map from the joint probability distribution function to the s-particle distribution functions is given by

$$f_s(x_1, p_1, \ldots, x_s, p_s) = \frac{n!}{(n-s)!} \int d^3x_{s+1} d^3p_{s+1} \ldots d^3x_N d^3p_N \; \rho(x_1, p_1, \ldots, x_N, p_N). \tag{4.1.7}$$

The time evolution of f_s depends on f_{s+1}. For example, the first two equations of the BBGKY hierarchy are

$$\frac{\partial f_1}{\partial t} + p_1 \cdot \frac{\partial f_1}{\partial x_1} = \int d^3x_2 d^3p_2 \; \frac{\partial \phi(|x_1 - x_2|)}{\partial x_1} \cdot \frac{\partial f_2}{\partial p_1}, \tag{4.1.8a}$$

$$\begin{aligned} &\frac{\partial f_2}{\partial t} + p_1 \cdot \frac{\partial f_2}{\partial x_1} + p_2 \cdot \frac{\partial f_2}{\partial x_2} - \frac{\partial \phi(|x_1 - x_2|)}{\partial x_1} \cdot \left(\frac{\partial f_2}{\partial p_1} - \frac{\partial f_2}{\partial p_2} \right) \\ &\qquad = \int d^3x_3 d^3p_3 \; \frac{\partial \phi(|x_1 - x_3|)}{\partial x_1} \cdot \frac{\partial f_3}{\partial p_1} + \frac{\partial \phi(|x_2 - x_3|)}{\partial x_2} \cdot \frac{\partial f_3}{\partial p_2}. \end{aligned} \tag{4.1.8b}$$

In [126], Marsden, Morrison and Weinstein described a construction where the space of BBGKY distribution functions $(f_1, f_2, \ldots, f_N)$ is the dual $\mathfrak{a}^*$ to a hierarchy Lie algebra $\mathfrak{a} = A_1 \oplus \ldots \oplus A_N$ satisfying $[A_a, A_b] \subset A_{a+b-1}$, with each component A_s corresponding to the s-particle distribution function f_s. They also showed that the BBGKY equations (4.1.8a,b, ...) form a noncanonical Hamiltonian system given by the Lie–Poisson bracket on $\mathfrak{a}^*$ and the Hamiltonian functional

$$\begin{aligned} H_{BBGKY} = &\int d^3x_1 d^3p_1 \; \frac{|p|^2}{2} f_1(x_1, p_1) \\ &+ \int d^3x_1 d^3p_1 d^3x_2 d^3p_2 \; \frac{\phi(|x_1 - x_2|)}{2} f_2(x_1, p_1, x_2, p_2). \end{aligned} \tag{4.1.9}$$

In the same paper, the map (4.1.7) is shown to be the dual of a Lie algebra homomorphism, hence a Poisson map. The BBGKY Hamiltonian (4.1.9) pulls back to the N-particle Hamiltonian (4.1.4), so the "Hamiltonian reduction" from the N-particle kinetic formulation to the BBGKY hierarchy is exact.

It is difficult to justify the passage from the N-particle description to the BBGKY hierarchy as a genuine reduction, since the system has increased in size. However, the BBGKY hierarchy is convenient for studying the possibility of truncating at a small number of f_s, which leads to a much smaller system of evolution equations. In particular, certain scaling hypotheses allow us to approximate the f_2 term on the right-hand side of (4.1.8a) in terms of f_1. Two well-known examples are the *Boltzmann–Grad limit* [23, 31] and the *Vlasov limit* [24, 31, 37, 95]; we refer to the respective references for detailed discussions.

In the Hamiltonian context, we would like to know whether truncations of the form $(f_1, f_2, \ldots, f_N) \mapsto (f_1, f_2, \ldots, f_s)$ ($s \ll N$) correspond to Poisson maps between Poisson manifolds. In [126], it is shown that A_1 is a Lie subalgebra of $\mathfrak{a}$, but not $A_1 \oplus \ldots \oplus A_s$ ($s \geq 2$). So the only truncation that is a Poisson map is $\iota^* : (f_1, f_2, \ldots, f_N) \mapsto f_1$, the dual to the inclusion $\iota : A_1 \hookrightarrow \mathfrak{a}$. This truncation leads to 1-*particle kinetic theory*, where the dynamical variable is the 1-*particle distribution function* $f_1(x, p, t) \in A_1 = C^\infty(\mathbb{R}^6)$, the expected phase space density of gas particles (see section **2.6.3**). However, the BBGKY Hamiltonian (4.1.9) does not factor through the Poisson map $\iota^* : \mathfrak{a}^* \to C^\infty(\mathbb{R}^6)$. Nonetheless, by making the mean-field approximation

$$f_2(x_1, p_1, x_2, p_2) = f_1(x_1, p_1) f_1(x_2, p_2) \tag{4.1.10}$$

in the BBGKY Hamiltonian (4.1.9), we obtain an approximate Hamiltonian depending on f_1 only, so such a Hamiltonian would factor through ι^*. In fact, choosing $\phi = 0$ recovers the collisionless Boltzmann equation (2.6.48) and choosing $\phi(r) = e^2/4\pi r$ recovers the Vlasov–Poisson equation (2.6.49) in three dimensions, where e is the suitably rescaled charge of the particles. We have thus shown that 1-particle kinetic theory can be obtained from the BBGKY hierarchy through an approximate reduction of Hamiltonian systems.

We have thus completed the discussion on the kinetic descriptions of an ideal monatomic gas. The passage along the hierarchy of kinetic descriptions, from N-body to Liouville to BBGKY to 1-particle kinetic theory, is manifestly Hamiltonian, where the mean-field approximation (4.1.10) is needed in the last step. The rest of the chapter is devoted to the much more nuanced problem of reducing 1-particle kinetic theory to a macroscopic *hydrodynamic* description, where the ideal gas is described by fields depending on position x and time but not on the full phase-space distribution of momentum p. Common examples of such hydrodynamic variables are the mass density $\rho(x, t)$, the momentum density $m(x, t)$ and the entropy density $s(x, t)$ of the gas. In the absence of viscous effects and thermal diffusion, the ideal gas is described by the compressible Euler equations (see section **2.6.1**), which is also a noncanonical Hamiltonian system. Does an exact or approximate Hamiltonian passage exist? How do we treat the p-dependence in such a passage?

We will discover that these questions are intimately related to cotangent bundle structure of phase space $\mathbb{R}^6 = T^*\mathbb{R}^3$. For the rest of the chapter, we take an orientable Riemannian manifold M without boundary as the domain of the ideal gas, and take its phase space to be the cotangent bundle T^*M, unless otherwise specified. In this generalised setting, distribution functions are functions on T^*M, and hydrodynamic variables are sections of certain vector bundles over M. We are interested in investigating *closures* of kinetic theory, where a finite or infinite set of hydrodynamic variables replicate the kinetic description exactly or approximately, similar to our investigation of macroscopic models from kinetic ones for multibead-chain suspensions in Chapter **3**. We focus on 1-particle kinetic theory and drop the subscript 1 for the distribution function henceforth.

4.2 The raw moment closure problem

The *moment closure problem* is a well-known property in the kinetic theory of gases and plasmas, where there is no exact description by a finite number of hydrodynamic variables for a kinetic system. The classical example is the lack of finite closure for *raw moments* or *Vlasov moments*, which are hydrodynamic variables of the form $\int d^n p\, p \dots p f(x,p,t)$. In the context of noncanonical Hamiltonian mechanics, this difficulty arises because the kinetic-theory Hamiltonian (2.6.50) contains the term $\int dV\, (|p|^2/2) f$, which is incompatible with finite closure owing to properties of the cotangent bundle. The main references are [71, 72, 74, 129, 130, 172, 176, 189].

4.2.1 The symmetric Schouten bracket

Let M be the domain of the gas, which is an n-dimensional manifold, and T^*M its cotangent bundle, with bundle projection $\pi : T^*M \to M$. Consider a covering by coordinate patches U on M, and let $(x^1, \dots, x^n)$ be the coordinates for a point x on M. The coordinate patches T^*U then covers T^*M, with induced coordinates $(x^1, \dots, x^n, p_1, \dots, p_n)$ for a point $(x,p) \in T^*M$ ($x \in M, p \in T^*_x M$), where $p_i = \langle p, \partial/\partial x^i \rangle_{T_x M}$ are the components for the cotangent vector p. A *homogeneous fibrewise polynomial of degree a in p* is a function with a local expression $S^{i_1 \dots i_a}(x) p_{i_1} \dots p_{i_a}$ in any of the coordinate patches T^*U. It is straightforward to check that the local functions $S^{i_1 \dots i_a}(x)$ are components of a symmetric rank-$(a,0)$ tensor $S \in \Gamma(Sym^a TM)$. We introduce the notation $\mathfrak{S}_a(M) = \Gamma(Sym^a TM)$, or simply $\mathfrak{S}_a$ when no confusion can arise, for brevity.

Conversely, any symmetric rank-$(a,0)$ tensor gives rise to a homogeneous fibrewise polynomial of degree a in p by the above construction. We denote the fibrewise polynomial

on T^*M associated to the symmetric tensor S in a coordinate-free way as

$$S^{i_1\dots i_a}(x)p_{i_1}\dots p_{i_a} := \langle S, \otimes^a p\rangle \in C^\infty(T^*M). \tag{4.2.1}$$

For symmetric rank-$(1,0)$ tensors i.e. vector fields $u \in \mathrm{Vect}(M)$, we use the special notation $\langle u, p\rangle = u^i p_i$. For symmetric rank-$(0,0)$ tensors i.e. functions $g \in C^\infty(M)$, the corresponding monomial is simply $\pi^* g \in C^\infty(T^*M)$. The association $S \mapsto \langle S, \otimes^a p\rangle$ can be extended $\mathbb{R}$-linearly to an injective vector space mapping $\iota_{mom} : \mathfrak{S} = \oplus_{a=0}^\infty \mathfrak{S}_a \hookrightarrow C^\infty(T^*M)$, whose image is precisely the space of fibrewise polynomials in p.

The identification of the space of symmetric tensors $\mathfrak{S}$ with the space of fibrewise polynomials on T^*M induces a Poisson algebra structure on $\mathfrak{S}$ [156, 157, 189]. The commutative and associative multiplication is defined on the direct summands as $* : \mathfrak{S}_a \times \mathfrak{S}_b \to \mathfrak{S}_{a+b}$:

$$T * S := \iota_{mom}^{-1}\left(\langle T, \otimes^a p\rangle\langle S, \otimes^b p\rangle\right), \tag{4.2.2}$$

and extended $\mathbb{R}$-linearly to $\mathfrak{S}$. The term $\langle T, \otimes^a p\rangle\langle S, \otimes^a p\rangle$ is a homogeneous fibrewise polynomial of degree $a+b$, so it is in the image of ι_{mom} and corresponds to a unique symmetric rank-$(a+b,0)$ tensor $T * S$. We recognise the operation $*$ (4.2.2) as the symmetrised tensor product:

$$(T * S)^{i_1\dots i_a j_1\dots j_b} = T^{(i_1\dots i_a} S^{j_1\dots j_b)}, \tag{4.2.3}$$

where the curved brackets in the indices indicate the average over all $(a+b)!$ permutations of $i_1, \dots, i_a, j_1, \dots, j_b$. The Lie bracket $[\cdot,\cdot] : \mathfrak{S}_a \times \mathfrak{S}_b \to \mathfrak{S}_{a+b-1}$ is similarly defined and is known as the *symmetric Schouten bracket*[1]:

$$[T, S] = -\iota_{mom}^{-1}\left\{\langle T, \otimes^a p\rangle, \langle S, \otimes^b p\rangle\right\}, \tag{4.2.4}$$

where $\{\cdot,\cdot\}$ is the canonical Poisson bracket on T^*M. The term $\{\langle T, \otimes^a p\rangle, \langle S, \otimes^a p\rangle\}$ is a homogeneous fibrewise polynomial of degree $a+b-1$, so it is in the image of ι_{mom} and corresponds to a unique symmetric rank-$(a+b-1,0)$ tensor. An explicit formula for (4.2.4) is

$$[T, S]^{i_1\dots i_{a-1} i_b\dots i_{b-1} j} = aT^{k(i_{a-1}}\partial_k S^{i_b\dots i_{b-1} j)} - bS^{k(i_b\dots i_{b-1}}\partial_k T^{i_{a-1} j)}, \tag{4.2.5}$$

where $\partial_k = \partial/\partial x^k$. The partial derivative ∂_k in (4.2.5) can also be replaced by the Levi-Civita connection ∇_k for any Riemannian metric on M. The space $\mathfrak{S}$ equipped with the

[1]The sign convention for the symmetric Schouten bracket (4.2.4) is so chosen that it coincides with the usual Lie bracket for vector fields; see (4.2.6a) below.

symmetrised tensor product (4.2.2) and the symmetric Schouten bracket (4.2.4) is then manifestly a Poisson algebra. We will not make much use of the commutative multiplication on $\mathfrak{S}$ in the following. Instead, we focus on the Lie algebra structure on $\mathfrak{S}$. In particular, $\iota_{mom} : \mathfrak{S} \hookrightarrow C^\infty(T^*M)$ is a Lie algebra anti-homomorphism.

As $[\mathfrak{S}_a, \mathfrak{S}_b] \subset \mathfrak{S}_{a+b-1}$ and the symmetric Schouten bracket does not vanish in general, the only Lie subalgebras of $\mathfrak{S}$ of the form $\mathfrak{S}_0 \oplus \mathfrak{S}_a \oplus \ldots \oplus \mathfrak{S}_A$ ($A \geq 0$) are the abelian Lie algebra $\mathfrak{S}_0$ and the Lie algebra of *fibrewise affine functions* $\mathfrak{S}_0 \oplus \mathfrak{S}_1$. The latter Lie subalgebra is so named because it consists of functions of the form $\langle u, p\rangle + \pi^* g$ for vector fields u and functions g on M, which are affine in p. For vector fields u, v and functions g, h on M, we have the following identities:

$$\{\langle u, p\rangle, \langle v, p\rangle\} = -\langle \mathcal{L}_u v, p\rangle\,, \tag{4.2.6a}$$

$$\{\langle u, p\rangle, \pi^* g\} = -\pi^*(\mathcal{L}_u g)\,, \tag{4.2.6b}$$

$$\{\pi^* g, \pi^* h\} = 0, \tag{4.2.6c}$$

where $\mathcal{L}_u$ is the Lie derivative along u on M (see sections **2.3.1** and **2.3.2**), so the symmetric Schouten bracket (4.2.4) for two vector fields $[u, v]$ is the usual Lie bracket, and $[u, g] = \mathcal{L}_u g$ is the Lie derivative on functions. We immediately recognise $\mathfrak{S}_0 \oplus \mathfrak{S}_1$ as the semidirect product Lie algebra $\mathfrak{s}_0 = \mathrm{Vect}(M) \ltimes C^\infty(M)$ considered in section **2.6.1**, and that the restriction $\iota_{mom,0} : \mathrm{Vect}(M) \ltimes C^\infty(M) \hookrightarrow C^\infty(T^*M)$ given explicitly as $(u, g) \mapsto \langle u, p\rangle + \pi^* g$ is an anti-homomorphism of Lie algebras. This construction is described in [84, 86, 130] in the context of cotangent lifts and moment maps.

Other interesting identities for the symmetric Schouten bracket (4.2.4) include, for any $h \in C^\infty(M), u \in \mathrm{Vect}(M), S \in \mathfrak{S}_a$, that

$$[u, S] = \mathcal{L}_u S, \tag{4.2.7a}$$

$$([S, h])^{i_1 \ldots i_{a-1}} = a S^{i_1 \ldots i_{a-1} j} \nabla_j h \tag{4.2.7b}$$

$$([S, \tilde{g}])^{i_1 \ldots i_a j} = -2\nabla^{(j} S^{i_1 \ldots i_a)}, \tag{4.2.7c}$$

where $\alpha_1, \ldots, \alpha_{a-1} \in \Omega^1(M)$ are 1-forms, $\tilde{g}$ the inverse of the Riemannian metric g on M, and ∇ is the Levi-Civita connection of g. The centraliser of $\tilde{g}$ in $\mathfrak{S}$, i.e. the subspace defined by $[S, \tilde{g}] = 0$ is called the space of *Killing tensor fields* and is an object of much interest in differential geometry [14, 55, 165, 189]. We will not dwell on Killing tensor fields too much in the following, but the identity (4.2.7c) will be useful later.

4.2.2 The Kuperschmidt–Manin bracket and finite closure

Dualising the Lie algebra anti-homomorphism $\iota_{mom} : \mathfrak{S} \hookrightarrow C^\infty(T^*M)$ gives us a Poisson map $\iota^*_{mom} : C^\infty(T^*M) \to \mathfrak{S}^*$, where $\mathfrak{S}^*$ is endowed with the minus Lie–Poisson bracket. As a vector space, $\mathfrak{S}^*$ is the direct product $\Pi_{a=0}^\infty \mathfrak{S}^*_a$, with $\mathfrak{S}^*_a = \Gamma(Sym^a T^*M \otimes \wedge^n M)$ being the space of symmetric rank-$(0,a)$ tensor densities and the dual pairing being integration over M. Explicitly, a typical element of $\mathfrak{S}^*$ is an infinite tuple

$$\left(A^{(0)}, A^{(1)}, \ldots\right), \text{ with } A^{(a)} = {A^{(a)}}_{i_1 \ldots i_a} dx^{i_1} \otimes \ldots dx^{i_n} \otimes d^n x \in \Gamma(Sym^a T^*M \otimes \wedge^n M), \tag{4.2.8}$$

and the appropriate space of functionals $\mathcal{F}(\mathfrak{S}^*)$ is the space of sufficiently regular functionals that depend on a *finite* number of the $A^{(a)}$. The explicit expression for the Kuperschmidt–Manin bracket for two such functionals F, G is then

$$\{F, G\}_{KM} = -\sum_{a=0}^{\infty} \left\langle A^{(a)}, \sum_{b=0}^{a+1} \left[\frac{\delta F}{\delta A^{(b)}}, \frac{\delta G}{\delta A^{(a+1-b)}} \right] \right\rangle_{\mathfrak{S}_a}, \tag{4.2.9}$$

where $[\cdot, \cdot]$ is the symmetric Schouten bracket (4.2.4). The sum in (4.2.9) is always finite because F, G both depend only on a finite number of the $A^{(a)}$. The image of ι^*_{mom} corresponds to taking the *raw moments* or *Vlasov moments* [70, 72, 176, 176] of $f \in C^\infty(T^*M)$. Explicitly, we have $\iota^*_{mom}[f] = (A^{(0)}[f], A^{(1)}[f], \ldots)$, with the a^{th} component defined in terms of the dual pairing with $T \in \mathfrak{S}_a$ as

$$\left\langle A^{(a)}[f], T \right\rangle_{\mathfrak{S}_a} = \int_{T^*M} dV \; T^{i_1 \ldots i_a}(x) p_{i_1} \ldots p_{i_a} f(x,p). \tag{4.2.10}$$

In particular, we have the following coordinate expressions:

$$A^{(0)}[f] = \int d^n p \; f, \tag{4.2.11a}$$

$${A^{(1)}}_i[f] = \int d^n p \; p_i f, \tag{4.2.11b}$$

$${A^{(2)}}_{ij}[f] = \int d^n p \; p_i p_j f, \tag{4.2.11c}$$

$${A^{(3)}}_{ijk}[f] = \int d^n p \; p_i p_j p_k f, \tag{4.2.11d}$$

and so on. We recognise $\rho[f] = A^{(0)}[f]$ as the *mass density* of the gas and $m[f] = A^{(1)}[f]$ as the *momentum density* of the gas. These $A^{(a)}$ are hydrodynamic variables as they are tensor densities over M, and the map ι^*_{mom} taking the distribution function f to its raw moments leads to an exact Hamiltonian reduction of 1-particle kinetic theory to hydrodynamics, although with an infinite number of hydrodynamic variables.

To complete the reduction, we must check if the relevant Hamiltonian functionals factor through ι^*_{mom}. The Hamiltonian functional (2.6.47) that generates the collisionless Boltzmann equation on a Riemannian manifold M with metric g can be written as

$$H_{KT}[f] = \int dV \, \frac{g^{ij}p_i p_j}{2} f = \int d^n x \frac{g^{ij}{A^{(2)}}_{ij}[f]}{2} = \tilde{H}_{KT} \circ \iota^*_{mom}[f], \tag{4.2.12}$$

where $dV = d^n x d^n p$ is the symplectic volume element (2.3.16), so the collisionless Boltzmann equation (2.6.48) can be exactly reduced to a the system generated by $\tilde{H}_{KT}$ on $\mathfrak{S}^*$:

$$\frac{\partial {A^{(a)}}_{i_1 \ldots i_a}}{\partial t} + \nabla^j \left({A^{(a+1)}}_{i_1 \ldots i_a j} \right) = 0, \tag{4.2.13}$$

obtained from computing $\{F, \tilde{H}_{KT}\}_{KP}$ for arbitrary functionals F with the aid of (4.2.7c). Similarly, the Vlasov–Poisson Hamiltonian (2.6.50) can be written as $H_{VP} = \tilde{H}_{VP} \circ \iota^*_{mom}$, where

$$\tilde{H}_{VP}[A^{(0)}, A^{(2)}] = \int d^n x \left(\frac{g^{ij}{A^{(2)}}_{ij}}{2} + \frac{e}{2}\varphi[A^{(0)}] \right), \tag{4.2.14}$$

where $\varphi \in C^\infty(M)$ is the electric potential defined by

$$-\nabla_j \nabla^j \varphi = e \frac{A^{(0)}}{\mu}, \tag{4.2.15}$$

where the right-hand side should be interpreted as the ratio between the scalar density $A^{(0)}$ and the Riemannian volume element $\mu = \sqrt{\det g} d^n x$. If M is compact, we subtract a suitable constant from the right-hand side of (4.2.15) – this is equivalent to introducing a uniformly charged background to keep the system neutral overall. Similarly, the self-gravitating Hamiltonian (2.6.53) for a self-gravitating system is

$$\tilde{H}_{SG}[A^{(0)}, A^{(2)}] = \int d^n x \left(\frac{g^{ij}{A^{(2)}}_{ij}}{2} + \frac{\mathrm{G}}{2}\varphi_g[A^{(0)}] \right), \tag{4.2.16}$$

where $\varphi_G \in C^\infty(M)$ is the gravitational potential defined by

$$\nabla_j \nabla^j \varphi_g = \frac{A^{(0)}}{\mu}. \tag{4.2.17}$$

As noted in section **2.6.3**, the Vlasov–Poisson and self-gravitating Hamiltonians are related by the replacement of constants $e^2 \mapsto -\mathrm{G}$. The system generated by $\tilde{H}_{Vlasov}$ on $\mathfrak{S}^*$ is

$$\frac{\partial {A^{(a)}}_{i_1 \ldots i_a}}{\partial t} + \nabla^j \left({A^{(a+1)}}_{i_1 \ldots i_a j} \right) + ae \nabla_{(i_1} \varphi {A^{(a-1)}}_{i_2 \ldots i_a)} = 0, \tag{4.2.18}$$

where for $a = 0$ the term depending on φ vanishes, so the ill-defined term $A^{(-1)}$ does not matter.

For both the collisionless Boltzmann and the Vlasov systems, an exact Hamiltonian reduction from 1-particle kinetic theory to a hydrodynamic description in terms of raw moments (4.2.10) is possible, since the respective Hamiltonian functionals factors through the distribution-to-moments map ι^*_{mom}. However, we have to keep all raw moments. The easiest way to see this is that both governing equations (4.2.13, 4.2.18) exhibit what is known as the *moment closure problem* – the time evolution of $A^{(a)}$ depends on $A^{(a+1)}$, so there is no finite subset of the $A^{(a)}$ equations that forms a closed system of evolution equations.

The moment closure problem is intimately related to the properties of the Kuperschmidt–Manin bracket (4.2.9). If F, G are functionals of $A^{(0)}, A^{(1)}$ only, then $\{F, G\}_{KM}$ is also a functional of $A^{(0)}, A^{(1)}$ only. However, if F, G are functionals of $A^{(0)}, A^{(1)}, A^{(2)}$ only, then

$$\{F, G\}_{KM} = K\left[A^{(0)}, A^{(1)}, A^{(2)}\right] - \left\langle A^{(3)}, \left[\frac{\delta F}{\delta A^{(2)}}, \frac{\delta G}{\delta A^{(2)}}\right]\right\rangle_{\mathfrak{S}_2}, \tag{4.2.19}$$

where K is some functional of $A^{(0)}, A^{(1)}, A^{(2)}$ only, so their Poisson bracket $\{F, G\}_{KM}$ now depends on $A^{(3)}$. Restating this in more abstract language, the space of functionals $\mathcal{F}(\mathfrak{S}^*_0 \oplus \mathfrak{S}^*_1)$ form a Poisson subalgebra of $\mathcal{F}(\mathfrak{S}^*)$, but the space $\mathcal{F}(\mathfrak{S}^*_0 \oplus \mathfrak{S}^*_1 \oplus \mathfrak{S}^*_2)$ does not form a Poisson subalgebra. More generally, since the only Lie subalgebras of $\mathfrak{S}$ of the form $\oplus^A_{a=0}\mathfrak{S}_a$ are when $A = 0$ or 1, these are also the only cases where the truncation maps $\mathfrak{S}^* \to \oplus^A_{a=0}\mathfrak{S}^*_a$ (i.e. projection to the first A components) are Poisson maps, and hence also the only cases where the multiplicative subalgebras $\mathcal{F}(\oplus^A_{a=0}\mathfrak{S}^*_a) \subset \mathcal{F}(\mathfrak{S}^*)$ are Poisson subalgebras. Since both the collisionless Boltzmann (4.2.12) and Vlasov–Poisson Hamiltonians (4.2.14) depend on $A^{(2)}$, we do not have a moment truncation that leads to a reduced Hamiltonian system with a finite number of hydrodynamic variables without making any extra uncontrolled approximations.

One recent approach in resolving the moment closure problem in the Hamiltonian framework, which has some success for the Vlasov–Poisson equation in one spatial dimension, is to assume a *closure relation*

$$A^{(3)} = C^{(3)}\left[A^{(0)}, A^{(1)}, A^{(2)}\right] \tag{4.2.20}$$

for the second term in (4.2.19) [145, 170, 171, 172]. Similarly, if one wishes to keep moments up to order s, one has to assume closure relations $A^{(b)} = C^{(b)}[A^{(0)}, \dots A^{(s)}]$ for $b = s+1, \dots, 2s-1$. This is an approximate Hamiltonian reduction by constructing a new Poisson bracket on the space $\mathfrak{S}^*_0 \oplus \mathfrak{S}^*_1 \oplus \mathfrak{S}^*_2$ (see section **2.5.5** for the mathematical

interpretation of such Hamiltonian reductions). This uncontrolled approximation transforms the moment system for the collisionless Boltzmann equation (4.2.13) into

$$\frac{\partial A^{(0)}}{\partial t} + \nabla^j \left({A^{(1)}}_j \right) = 0, \tag{4.2.21a}$$

$$\frac{\partial {A^{(1)}}_i}{\partial t} + \nabla^j \left({A^{(2)}}_{ij} \right) = 0 \tag{4.2.21b}$$

$$\frac{\partial {A^{(2)}}_{ik}}{\partial t} + \nabla^j \left({C^{(3)}}[A^{(0)}, A^{(1)}, A^{(2)}]_{ikj} \right) = 0, \tag{4.2.21c}$$

and similarly for the moment system of the Vlasov–Poisson equation (4.2.18), leading to a closed and finite system of moment equations. However, we cannot say that (4.2.21a-c) is a Hamiltonian system unless we have verified the Jacobi identity for the bracket (4.2.19) with the substitution (4.2.20). The author is unaware of general mathematical theories for identifying such closure relations that result in Poisson brackets – it would be interesting if a method for checking algebraic closure relations such as

$${C^{(3)}}_{ikj} = \frac{{A^{(1)}}_{(i}{A^{(1)}}_k{A^{(1)}}_{j)}}{A^{(0)}A^{(0)}} + \frac{{A^{(1)}}_{(i}{A^{(2)}}_{kj)}}{A^{(0)}} \tag{4.2.22}$$

exists, without resorting to verifying the Jacobi identity explicitly.

The more classical approach to the moment closure problem in the Hamiltonian framework is to make the uncontrolled approximation in the Hamiltonian functional. In particular, we make use of the Poisson map $\iota^*_{mom,0} : C^\infty(T^*M) \to \mathfrak{S}^*_0 \oplus \mathfrak{S}^*_1$ taking the distribution function f to only the first two moments (4.2.11a, 4.2.11b) [84, 129, 130]. If we make an ansatz of the form

$$g^{ij}{A^{(2)}}_{ij} = \frac{g^{ij}{A^{(1)}}_i{A^{(1)}}_j}{A^{(0)}} + 2V(A^{(0)}) \tag{4.2.23}$$

in the collisionless Boltzmann Hamiltonian (4.2.12), where $V : \mathbb{R} \to \mathbb{R}$ is a real function, then the new approximate Hamiltonian factors through $\iota^*_{mom,0}$ and the reduced Hamiltonian system is precisely the compressible Euler equations with constant entropy (see section **2.6.1.2**). The problem with this is that we have no physical grounds to justify the ansatz (4.2.23), except for the fact that it gives the right answer! In section **4.3** we identify a new family of hydrodynamic variables known as *generalised entropies*, and in section **4.4** we find a more physically justifiable ansatz than (4.2.23) that gives us the compressible Euler equations with non-constant entropy (see section **2.6.1**).

4.3 Poisson maps with entropy variables

In this section we describe an alternative set of hydrodynamic variables for the 1-particle distribution function which we call *generalised entropies*, and construct a family of Poisson

maps $\mathcal{J}_A (A = 0, 1, \ldots)$ from the space $C^\infty(T^*M)_+$ of positive distribution functions to the space $\mathfrak{s}_A^* = \mathrm{Vect}^*(M) \times \Omega^n(M, \mathbb{R}^{A+1})$ (see sections **2.6.1** and **2.6.3** for their definitions). Recall that the space $\mathfrak{s}_A^*$ of hydrodynamic variables consists of elements of the form $(m, (s_0, \ldots, s_A))$, where $m = m_i dx^i \otimes d^n x$ is the momentum density, $s_0 = s_0 d^n x$ is the mass density, $s_1 = s_1 d^n x$ is the entropy density, and $s_a = s_a d^n x$ for $a \geq 2$ are additional hydrodynamic variables that we notionally call *generalised entropy densities*. The map $\mathcal{J}_A : C^\infty(T^*M)_+ \to \mathfrak{s}_A^*$ is defined by the dual pairing

$$\langle \mathcal{J}_A[f], (u, (g_0, \ldots, g_A)) \rangle_{\mathfrak{s}_A} = \int_{T^*M} d^n x d^n p \, \left(\langle u, p \rangle f + \sum_{a=0}^{A} f (\log f)^a g_a \right). \tag{4.3.1}$$

In components, we have $\mathcal{J}_A[f] = (m_i[f] dx^i \otimes d^n x, (s_0[f] d^n x, \ldots, s_A[f] d^n x))$, where

$$m_i[f] = \int d^n p \, p_i f, \quad s_a[f] = \int d^n p \, f (\log f)^a \tag{4.3.2}$$

are the *momentum density* and the *generalised entropy densities* of the distribution function, respectively, obtained by integrating along the cotangent fibres i.e. integrating over p. In particular, $s_0[f]$ is the mass density and $s_1[f]$ is the spatial density of the Boltzmann entropy $f \log f$.[2]

Proposition 4.1. *The map $\mathcal{J}_A : C^\infty(T^*M)_+ \to \mathfrak{s}_A^*$ (4.3.1) is a Poisson map from the space of positive 1-particle distribution functions $C^\infty(T^*M)_+$ to the space $\mathfrak{s}_A^*$ of hydrodynamic variables with generalised entropy densities [42].*

The map $\mathcal{J}_0 : C^\infty(T^*M)_+ \to \mathfrak{s}_0^*$ takes the zeroth and first raw moments of f and coincides with the map $\iota_{mom,0}^* : C^\infty(T^*M) \to \mathfrak{S}_0^* \oplus \mathfrak{S}_1^*$ considered in section **4.2**. Unlike the map from distribution functions to raw moments, we can truncate this map at an arbitrary value of A and still have a Poisson map. Taking the p-integral of the Boltzmann entropy $f \log f$ is also somewhat considered in [80, 143], and Proposition 4.1 settles this as a component of a Poisson map.

Proof. Define the functions $y_a(z) : \mathbb{R}_+ \to \mathbb{R}$ for $a = 0, 1, 2, \ldots$ as

$$y_a(z) = z(\log z)^a. \tag{4.3.3}$$

We set $(\log z)^0 = 1$ by convention so that $y_0(z) = z$, and also set $y_a = 0$ for $a < 0$. These functions have removable singularities at $z = 0$ for $a \geq 1$. Each generalised entropy density

[2] We use the mathematician's sign convention for entropy in this chapter, so that the Boltzmann entropy is $f \log f$ and not $-f \log f$. The mathematician's sign convention is common in gas kinetic theory while the opposite physicist's sign convention is more popular in other areas of physics such as statistical mechanics and thermodynamics.

$s_a[f]$ can be written in terms of the y_a as $s_a[f] = \int d^n p\, y_a(f)$. The functions $y_a(z)$ satisfy the recurrence relations

$$z\frac{dy_a}{dz} - y_a = a y_{a-1}, \tag{4.3.4a}$$

$$z\frac{d^2 y_a}{dz^2} = a\frac{dy_{a-1}}{dz}. \tag{4.3.4b}$$

Now suppose we have functionals $\tilde{F}, \tilde{G} \in \mathcal{F}(C^\infty(T^*M)_+)$ such that $\tilde{F} = F \circ \mathcal{G}_A$ and $\tilde{G} = G \circ \mathcal{G}_A$ for some $F, G \in \mathcal{F}(\mathfrak{s}_A^*)$. To prove that

$$\left\{\tilde{F}, \tilde{G}\right\}_{KT} = \{F, G\}_{\mathfrak{s}_A^*} \circ \mathcal{G}_A, \tag{4.3.5}$$

we need to compute the functional derivative of $\tilde{F} = F \circ \mathcal{G}_A$. The functional chain rule gives

$$\left\langle \frac{\delta \tilde{F}}{\delta f}, \delta f \right\rangle_{C^\infty(T^*M)} = \left\langle \frac{\delta F}{\delta m}, \delta m[f] \right\rangle_{\mathrm{Vect}(M)} + \sum_{a=0}^{A} \left\langle \frac{\delta F}{\delta s_a}, \delta s_a[f] \right\rangle_{C^\infty(M)}, \tag{4.3.6}$$

and

$$\delta m[f] = d^n x \int d^n p\, p \delta f, \quad \delta s_a[f] = d^n x \int d^n p\, y_a'(f) \delta f. \tag{4.3.7}$$

Comparing both expressions gives

$$\frac{\delta \tilde{F}}{\delta f} = \left\langle \frac{\delta F}{\delta m}, p \right\rangle + \sum_{a=0}^{A} y_a'(f) \frac{\delta F}{\delta s_a}. \tag{4.3.8}$$

We have suppressed the pullback π^* of the cotangent bundle projection for notational simplicity. Here $\delta F/\delta m$ is a vector field on M, and $\delta F/\delta s_a$ is a function on M for each a, so they all depend on x only. Now we compute

$$\begin{aligned}
\left\{\tilde{F}, \tilde{G}\right\}_{KT} &= \int dV\, f \left\{ \frac{\delta \tilde{F}}{\delta f}, \frac{\delta \tilde{G}}{\delta f} \right\} \\
&= \int dV\, f \left\{ \left\langle \frac{\delta F}{\delta m}, p \right\rangle, \left\langle \frac{\delta G}{\delta m}, p \right\rangle \right\} \\
&\quad + \sum_{a=1}^{A} f \left\{ y_a'(f) \frac{\delta F}{\delta s_a}, \left\langle \frac{\delta G}{\delta m}, p \right\rangle \right\} + \sum_{b=1}^{A} f \left\{ \left\langle \frac{\delta F}{\delta m}, p \right\rangle, y_b'(f) \frac{\delta G}{\delta s_b} \right\} \\
&\quad + \sum_{a,b=1}^{A} f \left\{ y_a'(f) \frac{\delta F}{\delta s_a}, y_b'(f) \frac{\delta G}{\delta s_b} \right\}.
\end{aligned} \tag{4.3.9}$$

Using (4.2.6a), the term on the first line of (4.3.9) is

$$\int dV\ f\left\{\left\langle\frac{\delta F}{\delta m},p\right\rangle,\left\langle\frac{\delta G}{\delta m},p\right\rangle\right\}=-\int dV\ f\left\langle\left[\frac{\delta F}{\delta m},\frac{\delta G}{\delta m}\right],p\right\rangle,$$
$$=-\left\langle m[f],\left[\frac{\delta F}{\delta m},\frac{\delta G}{\delta m}\right]\right\rangle_{\mathrm{Vect}(M)}. \tag{4.3.10}$$

The second line of (4.3.9) contains two similar groups of terms. We compute one of them as follows:

$$\begin{aligned}
&\int dV\ f\left\{y_a'(f)\frac{\delta F}{\delta s_a},\left\langle\frac{\delta G}{\delta m},p\right\rangle\right\}\\
&=\int dV\ \left(fy_a'(f)\left\{\frac{\delta F}{\delta s_a},\left\langle\frac{\delta G}{\delta m},p\right\rangle\right\}+fy_a''(f)\frac{\delta F}{\delta s_a}\left\{f,\left\langle\frac{\delta G}{\delta m},p\right\rangle\right\}\right),\\
&=\int dV\left((y_a(f)+ay_{a-1}(f))\left\{\frac{\delta F}{\delta s_a},\left\langle\frac{\delta G}{\delta m},p\right\rangle\right\}+\frac{\delta F}{\delta s_a}\left\{ay_{a-1}(f),\left\langle\frac{\delta G}{\delta m},p\right\rangle\right\}\right),\\
&=\int dV\left((y_a(f)+ay_{a-1}(f))\left\{\frac{\delta F}{\delta s_a},\left\langle\frac{\delta G}{\delta m},p\right\rangle\right\}-ay_{a-1}(f)\left\{\frac{\delta F}{\delta s_a},\left\langle\frac{\delta G}{\delta m},p\right\rangle\right\}\right),\\
&=\int dV\ y_a(f)\left(\mathcal{L}_{\frac{\delta G}{\delta m}}\frac{\delta F}{\delta s_a}\right)=\left\langle s_a[f],\mathcal{L}_{\frac{\delta G}{\delta m}}\frac{\delta F}{\delta s_a}\right\rangle_{C^\infty(M)}.
\end{aligned}\tag{4.3.11}$$

We have used the identity (2.1.3), Lemma 2.1 and the recurrence relations (4.3.4a,b) to manipulate terms involving $y_a(f)$ and its derivatives in and out of the canonical Poisson bracket. The terms on the last line of (4.3.9) vanish, because

$$\begin{aligned}
&\int dV\ f\left\{y_a'(f)\frac{\delta F}{\delta s_a},y_b'(f)\frac{\delta G}{\delta s_b}\right\}\\
&=\int dV\ f\Bigg(y_a'(f)y_b'(f)\left\{\frac{\delta F}{\delta s_a},\frac{\delta G}{\delta s_b}\right\}+y_a'(f)\frac{\delta G}{\delta s_b}\left\{\frac{\delta F}{\delta s_a},y_b'(f)\right\}\\
&\qquad\qquad+\frac{\delta F}{\delta s_a}y_b'(f)\left\{y_a'(f),\frac{\delta G}{\delta s_b}\right\}+\frac{\delta F}{\delta s_a}\frac{\delta G}{\delta s_b}\left\{y_a'(f),y_b'(f)\right\}\Bigg)\\
&=\int dV\ f\left(y_a'(f)\frac{\delta G}{\delta s_b}\left\{\frac{\delta F}{\delta s_a},y_b'(f)\right\}+\frac{\delta F}{\delta s_a}y_b'(f)\left\{y_a'(f),\frac{\delta G}{\delta s_b}\right\}\right)\\
&=\int dV\ \left(fy_a'(f)y_b''(f)\frac{\delta G}{\delta s_b}\left\{\frac{\delta F}{\delta s_a},f\right\}+fy_a''(f)y_b'(f)\frac{\delta F}{\delta s_a}\left\{f,\frac{\delta G}{\delta s_b}\right\}\right)\\
&=\int dV\ \left(\frac{\delta G}{\delta s_b}\left\{\frac{\delta F}{\delta s_a},I_{ab}(f)\right\}+\frac{\delta F}{\delta s_a}\left\{I_{ba}(f),\frac{\delta G}{\delta s_b}\right\}\right)\\
&=-\int dV\ \left(I_{ab}(f)+I_{ba}(f)\right)\left\{\frac{\delta F}{\delta s_a},\frac{\delta G}{\delta s_b}\right\}=0.
\end{aligned}\tag{4.3.12}$$

We have $\{\delta F/\delta s_a,\delta G/\delta s_b\}=0$ because both arguments are functions of x only. The function $I_{ab}(z)$ introduced on the second-to-last line of (4.3.12) is an antiderivative to

$zy'_a(z)y''_b(z)$:[3]

$$I_{ab}(z) = \int_0^z dw\ w y'_a(w) y''_b(w). \tag{4.3.13}$$

Putting everything together, we have

$$\begin{aligned}\left\{\tilde{F}, \tilde{G}\right\}_{KT} = &- \left\langle m[f], \left[\frac{\delta F}{\delta m}, \frac{\delta G}{\delta m}\right]\right\rangle_{\mathrm{Vect}(M)} \\ &- \sum_{a=0}^{A} \left\langle s_a[f], \mathcal{L}_{\frac{\delta F}{\delta m}} \frac{\delta G}{\delta s_a} - \mathcal{L}_{\frac{\delta G}{\delta m}} \frac{\delta F}{\delta s_a} \right\rangle_{C^\infty(M)},\end{aligned} \tag{4.3.14}$$

which is precisely the $(-)$-Lie–Poisson bracket on $\mathfrak{s}_A^*$ (2.6.5), evaluated at the image of the Poisson map $\mathcal{J}_A[f] = (m[f], (s_0[f], \ldots, s_A[f]))$. □

The Poisson manifolds $C^\infty(T^*M)_+$ and $\mathfrak{s}_A^*$ are linear, in the sense that they are open subsets of vector spaces and that the Poisson brackets are linear. However, the Poisson map $\mathcal{J}_A$ is genuinely nonlinear. The rest of the section is devoted to discussing the mathematical properties of $\mathcal{J}_A$.

4.3.1 Properties of $\mathcal{J}_A$

The nonlinearities in $\mathcal{J}_A$ arise naturally from considering the *generalised eigenvalue-eigenvector problem* [11]

$$\left(z\frac{d}{dz} - \lambda\right)^A y(z) = 0 \tag{4.3.15}$$

of the Euler operator on the positive real axis $z(d/dz) : C^\infty(\mathbb{R}_+) \to C^\infty(\mathbb{R}_+)$. The vector space of solutions to (4.3.15) is denoted V_λ^A. Solving the generalised eigenvalue-eigenvector problem (4.3.15) gives us a characterisation of V_λ^A as

$$V_\lambda^A = \mathrm{span}\left(z^\lambda, z^\lambda \log z, \ldots z^\lambda (\log z)^A\right), \tag{4.3.16}$$

which in particular shows that there is a chain of inclusions

$$0 \subset V_\lambda^0 \subset V_\lambda^1 \subset \ldots \subset V_\lambda^A, \tag{4.3.17}$$

with the dimension increasing by 1 in each inclusion. Such a chain (4.3.17) is called a *complete flag*. Moreover, for each $a = 0, \ldots, A$, we have

$$(z(d/dz) - 1)V_\lambda^a \subset V_\lambda^{a-1} \quad \text{(set } V_\lambda^{-1} = 0 \text{ by convention)}. \tag{4.3.18}$$

[3] We can express $zy'_a(z)y''_b(z)$ as a polynomial in $\log z$, so the integral (4.3.13) converges and $I_{ab}(z)$ is a linear combination of $z(\log z)^c$ for suitable integers c.

We immediately recognise the functions $y_0(z), \ldots, y_A(z)$ (4.3.3) as an ordered basis for V_1^A. The nonlinear components of $\mathcal{J}_A$ then correspond to the generalised eigenvectors $y_1(z), \ldots, y_A(z)$, which is a natural extension of the ordinary eigenvector $y_0(z) = z$ that gives a linear component.

Given a complete flag $0 \subset V_1^0 \subset V_1^1 \subset \ldots \subset V_1^A$ of generalised eigenspaces, it is natural to consider the group of unipotent[4] linear transformations that preserve the flag. In the ordered basis $y_0(z), \ldots, y_A(z)$, these unipotent transformations are precisely the matrices of the from $I + \Lambda$, where Λ is a strictly upper triangular matrix. The physical origin of these transformations is the *change of action scale* in f. The true dimensionless expression for $\log f$ is $\log(h^n f)$, where h is an arbitrary "Planck's constant" that defines an action ($[xp]$) scale. This arbitrary action scale, which can only be determined as the true Planck's constant in quantum or semiclassical treatments, leads to integration constants in many expressions in classical thermodynamics [103]. Changes in the reference action scale leads to transformations of the form $\log z \mapsto \log z + \Lambda$ in the definitions (4.3.3) of $y_a(z)$. Let us also allow for a different change of scale for each occurrence of $\log z$ in (4.3.3), for example $z(\log z)^2$ to $z(\log z + \Lambda_1)(\log z + \Lambda_2)$. The general form of such a transformation is

$$\tilde{y}_a = y_a(z) + \sum_{b<a} y_b(z)\Lambda_{ba}, \tag{4.3.19}$$

where Λ_{ba} is a strictly upper-triangular $(A+1) \times (A+1)$ matrix of constants, i.e. $\Lambda_{ba} = 0$ if $b \geq a$. The induced transformation $s_a[f] \mapsto \tilde{s}_a[f]$ on the generalised entropy densities is

$$\tilde{s}_a = s_a + \sum_{b<a} s_b \Lambda_{ba}, \tag{4.3.20}$$

which is a Poisson automorphism of $\mathfrak{s}_A^*$. The transformation (4.3.20) adds constant multiples of the lower generalised entropy densities to the higher generalised entropy densities. The $a = 1$ case of (4.3.20) reflects that the specific entropy $\eta_1 = s_1/s_0$ is only uniquely specified up to a global constant in classical thermodynamics.

4.3.2 A Poisson map involving a formal parameter

One strategy for solving the generalised eigenvalue-eigenvector problem (4.3.15) is to solve an ordinary eigenvalue-eigenvector problem for the *generating function*

$$\left(z\frac{d}{dz} - (1+\xi)\right) y(z,\xi) = 0, \tag{4.3.21}$$

[4]A matrix L is *unipotent* if $(L-I)^k = 0$ for all sufficiently large integers k.

where ξ is a formal parameter. Expanding $y(z,\xi) = \sum_{a=0}^{\infty} y_a(z)\xi^a/a!$ gives the equations

$$\left(z\frac{d}{dz} - 1\right) y_a(z) = a y_{a-1}(z), \tag{4.3.22}$$

(cf. (4.3.4a)) which leads to a family of generalised eigenvectors $y_a \in V_1^a \setminus V_1^{a-1}$. The solution to (4.3.21) is of course $z^{1+\xi}$, which is the generating function for our functions $y_a(z) = z(\log z)^a$. This leads us to consider whether there are Poisson maps containing the component $f^{1+\xi}$ whose truncated power series in ξ yields the Poisson maps $\mathcal{J}_A$ – we answer this positively in this section.

Consider the *path space* $PC^\infty(M)$ *of one-parameter families of functions on* M. The elements of $PC^\infty(M)$ are maps $g_\xi : I \to C^\infty(M)$. The Lie algebra of vector fields $\mathrm{Vect}(M)$ has a representation on $PC^\infty(M)$ by acting on the image. More explicitly, the action of a vector field u on g_ξ is $g_\xi \mapsto \mathcal{L}_u g_\xi$. This gives rise to a semidirect product Lie algebra $\mathrm{Vect}(M) \ltimes PC^\infty(M)$.

We take the smooth dual space to this semidirect product Lie algebra to be $\mathrm{Vect}(M)^* \times P\Omega^n(M)$, where $P\Omega^n(M)$ is the *path space* $P\Omega^n(M)$ *of top-degree forms (or densities) on* M, i.e. the space of one-parameter families of n-forms $\rho_\xi : I \to \Omega^n(M)$. The dual pairing between $P\Omega^n(M)$ and $PC^\infty(M)$ is given by integration over $I \times M$, where I is equipped with the standard measure $d\xi$. Consider the map $\mathsf{J} : C^\infty(T^*M)_+ \to \mathrm{Vect}(M)^* \times P\Omega^n(M)$, defined by

$$\langle \mathsf{J}[f], (u, g_\xi)\rangle = \int_{T^*M} dV \ \left(\langle u, p\rangle f + \int_I d\xi \ \left(f^{1+\xi} g_\xi\right)\right). \tag{4.3.23}$$

In components, we have $\mathsf{J}[f] = (m_i[f]dx^i \otimes d^n x, \rho_\xi[f] d^n x)$, where

$$m_i[f] = \int d^n p \; p_i f, \quad \rho_\xi[f] = \int d^n p \; f^{1+\xi}. \tag{4.3.24}$$

The quantity ρ_ξ is the spatial density of the so-called *Tsallis entropy*[5] [178] up to a multiplicative constant. For sufficiently regular and decaying f, the integrals in the definition of $\mathsf{J}[f]$ are finite for all ξ in some interval I containing 0. We claim that

Proposition 4.2. *The map* $\mathsf{J} : C^\infty(T^*M)_+ \to \mathrm{Vect}(M)^* \times P\Omega^n(M)$ *(4.3.23) is a Poisson map.*

Proof. Consider $\tilde{F}, \tilde{G} \in \mathcal{F}(C^\infty(T^*M)_+)$ such that $\tilde{F} = F \circ \mathsf{J}$ and $\tilde{G} = G \circ \mathsf{J}$ for some $F, G \in \mathcal{F}(\mathrm{Vect}(M)^* \times P\Omega^n(M))$. We wish to check

$$\left\{\tilde{F}, \tilde{G}\right\}_{KT} = \{F, G\}_{\mathrm{Vect}(M)^* \times P\Omega^n(M)} \circ \mathsf{J} \tag{4.3.25}$$

[5]Note that ρ_ξ is not a fractional density despite being a p-integral of $f^{1+\xi}$. In terms of the density $\psi = f dV$, the expression to be integrated is $\psi(\psi/dV)^\xi$.

by direct computation. The functional chain rule gives

$$\frac{\delta \tilde{F}}{\delta f} = \left\langle \frac{\delta F}{\delta m}, p \right\rangle + \int_I d\xi \; (1+\xi) f^\xi \frac{\delta F}{\delta \rho_\xi}, \tag{4.3.26}$$

and similarly for $\tilde{G}$. Since integration in ξ can be pulled out of the canonical Poisson bracket, we can separate $\{\tilde{F}, \tilde{G}\}_{KT}$ into three groups of terms, each with $0, 1$ or 2 ξ-integrals respectively. The first group of terms with no ξ-dependence is just $-\langle m[f], [\delta F/\delta m, \delta G/\delta m]\rangle$. For the second group of terms with a single ξ-integral, we compute one of them as

$$\begin{aligned}
&\int_I d\xi \int dV \; f \left\{ (1+\xi) f^\xi \frac{\delta F}{\delta \rho_\xi}, \left\langle \frac{\delta G}{\delta m}, p \right\rangle \right\} \\
&= \int_I d\xi \int dV \; (1+\xi) \left(f^{1+\xi} \left\{ \frac{\delta F}{\delta \rho_\xi}, \left\langle \frac{\delta G}{\delta m}, p \right\rangle \right\} + f \frac{\delta F}{\delta \rho_\xi} \left\{ f^\xi, \left\langle \frac{\delta G}{\delta m}, p \right\rangle \right\} \right) \\
&= \int_I d\xi \int dV \; (1+\xi) f^{1+\xi} \left\{ \frac{\delta F}{\delta \rho_\xi}, \left\langle \frac{\delta G}{\delta m}, p \right\rangle \right\} + \frac{\delta F}{\delta \rho_\xi} \left\{ \xi f^{1+\xi}, \left\langle \frac{\delta G}{\delta m}, p \right\rangle \right\} \\
&= \int_I d\xi \int dV \; f^{1+\xi} \left\{ \frac{\delta F}{\delta \rho_\xi}, \left\langle \frac{\delta G}{\delta m}, p \right\rangle \right\}, \\
&= \int_I d\xi \; \left\langle \rho_\xi[f], \mathcal{L}_{\frac{\delta G}{\delta m}} \frac{\delta F}{\delta \rho_\xi} \right\rangle_{C^\infty(M)},
\end{aligned} \tag{4.3.27}$$

where we used Lemma 2.1 in the second-to-last line of (4.3.27). The other term is computed identically. The third group of terms vanishes:

$$\begin{aligned}
&\int_{I\times I} d\xi d\xi' \int dV \; (1+\xi)(1+\xi') f \left\{ f^\xi \frac{\delta F}{\delta \rho_\xi}, f^{\xi'} \frac{\delta G}{\delta \rho_{\xi'}} \right\} \\
&= \int_{I\times I} d\xi d\xi' \int dV \; (1+\xi)(1+\xi') \left(f^{1+\xi} \left\{ \frac{\delta F}{\delta \rho_\xi}, f^{\xi'} \right\} \frac{\delta G}{\delta \rho_{\xi'}} + f^{1+\xi'} \left\{ f^\xi, \frac{\delta G}{\delta \rho_{\xi'}} \right\} \frac{\delta F}{\delta \rho_\xi} \right) \\
&= \int_{I\times I} d\xi d\xi' \int dV \; \frac{(1+\xi)(1+\xi')}{1+\xi+\xi'} \left(\left\{ \frac{\delta F}{\delta \rho_\xi}, \xi' f^{1+\xi+\xi'} \right\} \frac{\delta G}{\delta \rho_{\xi'}} + \left\{ \xi f^{1+\xi+\xi'}, \frac{\delta F}{\delta \rho_\xi} \right\} \frac{\delta G}{\delta \rho_{\xi'}} \right) \\
&= 0,
\end{aligned} \tag{4.3.28}$$

using Lemma 2.1 and the fact that $\{\delta F/\delta \rho_\xi, \delta G/\delta \rho_{\xi'}\} = 0$ in the last line. Putting everything together, we have

$$\begin{aligned}
\left\{ \tilde{F}, \tilde{G} \right\}_{KT} = &- \left\langle m[f], \left[\frac{\delta F}{\delta m}, \frac{\delta G}{\delta m} \right] \right\rangle_{\mathrm{Vect}(M)} \\
&- \int_I d\xi \; \left\langle \rho_\xi[f], \mathcal{L}_{\frac{\delta F}{\delta m}} \frac{\delta G}{\delta \rho_\xi} - \mathcal{L}_{\frac{\delta G}{\delta m}} \frac{\delta F}{\delta \rho_\xi} \right\rangle_{C^\infty(M)},
\end{aligned} \tag{4.3.29}$$

which proves that J is indeed a Poisson map. □

Having constructed the Poisson map J, we proceed to construct the second Poisson map that would give $\mathcal{G}_A$ when composed to J. This second map arises from the theory of *jet spaces*, which codify Taylor expansions in a geometrical manner [109, 141]. Consider the sequence of projections

$$J_0^0(I,\Omega^n(M)) \leftarrow J_0^1(I,\Omega^n(M)) \leftarrow \ldots \leftarrow J_0^\infty(I,\Omega^n(M)) \leftarrow P\Omega^n(M), \tag{4.3.30}$$

where $J_0^A(I,\Omega^n(M))$ is the space of *A-jets of maps $\rho_\xi : I \to \Omega^n(M)$ at $\xi = 0$*, defined as the quotient space of $P\Omega^n(M)$ under the equivalence relation of agreement in Taylor series at $\xi = 0$ up to order A (see also section **3.3.1**). The *infinite jet space* $J_0^\infty(I,\Omega^n(M))$ is defined similarly, with the equivalent relation being the agreement in Taylor series up to arbitrary order. Each projection $J_0^A \to J_0^B$ for $A > B$ in (4.3.30) corresponds to a further truncation of the Taylor expansion of ρ_ξ.

To simplify notation, we use the shorthand V for $\mathrm{Vect}(M)$ and omit the arguments in the jet spaces for the rest of the section. We would like to show that the sequence of projections

$$\mathrm{V}^* \times J_0^0 \leftarrow \mathrm{V}^* \times J_0^1 \leftarrow \ldots \leftarrow \mathrm{V}^* \times J_0^\infty \leftarrow \mathrm{V}^* \times P\Omega^n(M) \tag{4.3.31}$$

are Poisson maps between Poisson manifolds, so that composing J with these projections corresponds to truncating the Taylor series of ρ_ξ, hence giving the Poisson map $\mathcal{G}_A$. This can be achieved by considering the spaces in (4.3.31) as smooth duals of Lie algebras and the maps as adjoints of injective Lie algebra homomorphisms. Consider the space of $C^\infty(M)$-valued distributions on I, which we denote by $D(I,C^\infty(M))$ or simply D for brevity. The Lie algebra V acts on D by Lie differentiation on its values: $g_\xi \mapsto \pounds_u g_\xi$, where u is a vector field and g_ξ is a $C^\infty(M)$-valued distribution. The subspace D_0^A of distributions that are supported at 0 and are of order at most A is invariant under this action. An element of D_0^A can always be written in the form

$$g_\xi = \sum_{a=0}^{A} g_a(-1)^a \frac{d^a}{d\xi^a}\delta(\xi), \quad \text{where } g_a \in C^\infty(M). \tag{4.3.32}$$

The subspace $D_0^\infty = \cup_{a=0}^\infty D_0^a$ is also invariant. The inclusions of these invariant subspaces induces a sequence of injective homomorphisms between semidirect product Lie algebras:

$$\mathrm{V} \ltimes D_0^0 \hookrightarrow \mathrm{V} \ltimes D_0^1 \hookrightarrow \ldots \hookrightarrow \mathrm{V} \ltimes D_0^\infty \hookrightarrow \mathrm{V} \ltimes D. \tag{4.3.33}$$

We recover the sequence (4.3.31) from dualising the sequence of injective homomorphisms between Lie algebras (4.3.33). This endows each space in (4.3.31) with a Lie–Poisson structure, and makes each map in (4.3.31) a Poisson map by being the adjoint of a Lie algebra homomorphism.

Now we can explain the connection between J and $\mathcal{G}_A$. Consider the isomorphism $D_0^A \simeq C^\infty(M, \mathbb{R}^{A+1})$ given by the map $g_\xi \mapsto (g_0, \ldots, g_A)$, where the g_a are as defined in (4.3.32). The action of V on D_0^A corresponds to componentwise Lie differentiation on $C^\infty(M, \mathbb{R}^{A+1})$ under this isomorphism. We can thus identify $\mathrm{V} \ltimes D_0^A$ with $\mathfrak{s}_A$ as semidirect product Lie algebras (see section **2.6.1**), and hence identify $\mathrm{V}^* \times J_0^A$ with $\mathfrak{s}_A^*$ as Poisson manifolds. The Poisson map $\mathcal{G}_A$ (4.3.1) is then recovered from composing J (4.3.23) with the sequence of projections (4.3.31). Indeed, the pairing of $\rho_\xi[f]$ with g_ξ in (4.3.32) is

$$\begin{aligned}\langle \rho_\xi[f], g_\xi \rangle_{PC^\infty(M)} &= \int_I d\xi \ \langle \rho_\xi[f], g_\xi \rangle_{C^\infty(M)} \,, \\ &= \int_I d\xi \ \sum_{a=0}^{A} (-1)^a \frac{d^a \delta(\xi)}{d\xi^a} \langle \rho_\xi[f], g_a \rangle_{C^\infty(M)} \,, \\ &= \sum_{a=0}^{A} \langle s_a[f], g_a \rangle_{C^\infty(M)} \,. \end{aligned} \tag{4.3.34}$$

The Poisson map J can be truncated at or expanded around other values of ξ with a similar reasoning as above, by considering distributions on I that are supported at a finite number of points $\xi_1, \ldots, \xi_k$, with prescribed finite order A_j at each point ξ_j. This creates a Poisson map from $C^\infty(T^*M)_+$ to $\mathfrak{s}_A^*$, where $A+1 = \sum_{j=1}^k (A_j + 1)$ is the number of $C^\infty(M)$-degrees of freedom. The components of such a Poisson map $J : C^\infty(T^*M)_+ \to \mathfrak{s}_A^*$ are given explicitly as

$$\begin{aligned} m_i[f] &= \int d^n p \ p_i f, \\ \rho_{\xi_j}^{(a)}[f] &= \int d^n p f^{1+\xi_j} (\log f)^a, \quad j = 1, \ldots, k, \ a = 0, \ldots, A_j. \end{aligned} \tag{4.3.35}$$

For example, if we take $k = 2$, $\xi_1 = 0$, $\xi_2 = \xi$ and $A_1 = A_2 = 0$, we obtain a Poisson map $J : C^\infty(T^*M)_+ \to \mathfrak{s}_1^*$ that takes f to $(m[f], \rho[f], \rho_\xi[f])$, where the role of the entropy density is now played by the Tsallis entropy (4.3.24).

Another example of such a Poisson map is $\mathcal{G}_A^{pol} : C^\infty(T^*M)_+ \to \mathfrak{s}_A^*$, where we take the ξ_j to be integers and the A_j to be zero:

$$\mathcal{G}_A^{pol}[f] = \Big(m_i[f] dx^i \otimes d^n x, (\rho_0^{pol}[f] d^n x, \ldots, \rho_A^{pol}[f] d^n x) \Big) \,, \tag{4.3.36}$$

where

$$m_i[f] = \int d^n p \ p_i f, \quad \rho_a^{pol}[f] = \int d^n p \ f^{1+a}. \tag{4.3.37}$$

The condition $f > 0$ can be relaxed for the map $\mathcal{G}_A^{pol}$, since positive integer powers of f are uniquely defined even when f is not positive. Thus we can extend the domain of $\mathcal{G}_A^{pol}$

to all of $C^\infty(T^*M)$. Moreover, since $\mathcal{J}_A^{pol}$ can be defined using only integer powers of f, the pullback $(\mathcal{J}_A^{pol})^* F$ of a *polynomial* functional F on $\mathfrak{s}_A^*$ is a polynomial functional on $C^\infty(T^*M)$. The maps $\mathcal{J}_A^{pol}$ (4.3.12) can be useful if one wishes to work in a purely algebraic setting (cf. sections **2.2.1** and **2.1.4**).

4.4 Fluid dynamics as a Hamiltonian approximation to kinetic theory

Having constructed the large family of Poisson maps $\mathcal{J}_A$ (4.3.1) and J (4.3.23) in section **4.3**, we return to investigate the respective Hamiltonian functionals in 1-particle kinetic theory and hydrodynamics with non-constant entropy. We find that kinetic-theory Hamiltonian does not factor through any of the Poisson maps we have constructed, again due to the presence of the $|p|^2$ term (4.2.12), so an exact Hamiltonian reduction is not possible. However, we can obtain an approximate Hamiltonian that factors through $\mathcal{J}_1$ by ignoring the contribution from the entropy of the distribution relative to its local Maxwellian. For the rest of this section, we revert to the more conventional notation for the mass density $\rho = s_0$ and the entropy density $s = s_1$. We focus on the cases $M = \mathbb{R}^n$ or $\mathbb{T}^n$, but the results can be adapted to general Riemannian manifolds by using the Riemannian inner product for vectors e.g. $|p|^2 \mapsto g^{ij} p_i p_j$ and inserting the Riemannian volume element $\mu = \sqrt{\det g_{ij}}\, d^n x$ at suitable places.

Consider a 1-particle distribution function $f = f(x,p)$ that describes the state of a monatomic ideal gas. We define the quantities

$$\rho[f] = \int d^n p\; f(x,p), \tag{4.4.1a}$$

$$m[f] = \int d^n p\; p f(x,p), \qquad u[f] = \frac{m[f]}{\rho[f]}, \tag{4.4.1b}$$

$$s[f] = \int d^n p\; f(x,p) \log f(x,p), \tag{4.4.1c}$$

$$\theta[f] = \frac{1}{n\rho} \int d^n p\; |p-u|^2 f(x,p), \tag{4.4.1d}$$

Here $(m[f], \rho[f], s[f])$ are the components of the Poisson map $\mathcal{J}_1 : C^\infty(T^*M)_+ \to \mathfrak{s}_1^*$, which we interpret as the momentum density, mass density and entropy density respectively, $u[f]$ is the mean velocity, and $\theta[f]$ is the *kinetic-theory temperature*. These quantities are all *hydrodynamic variables*. The spatial density of the energy of the ideal gas can be split into a mean part $\rho|u|^2/2$ corresponding to the kinetic energy of the mean motion of the particles,

and a thermal part $n\rho\theta/2$ corresponding to the kinetic energy of the motion of the particles relative to that mean. The splitting reads

$$H_{KT}[f] = \int dV\ \frac{|p|^2}{2} f = \int d^n x\ \left(\frac{|m[f]|^2}{2\rho[f]} + \frac{n}{2}\rho[f]\theta[f] \right). \tag{4.4.2}$$

A similar splitting also appears in the hydrodynamic description of the gas. The total energy density of the fluid (2.6.7) is split into a kinetic part $|m|^2/2\rho$ and a thermal part $\rho U(\rho, s)$, where $U(\rho, s)$ is the internal energy per unit mass of the fluid as determined by a thermodynamic equation of state. For a monatomic ideal gas, we have $U = (n/2)T$, where $T(\rho, s)$ is the *thermodynamic temperature* of the gas, defined implicitly by

$$\frac{s}{\rho} = \log\left(\rho T^{-n/2}\right) + C. \tag{4.4.3}$$

Here s/ρ is the local specific entropy, and C is an arbitrary constant. The Hamiltonian functional that generates the compressible Euler equations for a monatomic ideal gas is (2.6.7)

$$H_{fluids}[m, \rho, s] = \int d^n x\ \left(\frac{|m|^2}{2\rho} + \frac{n}{2}\rho T(\rho, s) \right), \tag{4.4.4}$$

where $T(\rho, s)$ is obtained from rearranging (4.4.3). Comparing (4.4.2) and (4.4.4), both Hamiltonians contain a kinetic part $|m|^2/2\rho$ and a thermal part. The kinetic parts agree under the Poisson map $\mathcal{J}_1$, so it is tempting to hope that the kinetic-theory temperature $\theta[f]$ can be described in terms of $(m[f], \rho[f], s[f])$, preferably through the equation of state $T(\rho, s)$. If this holds, H_{KT} would be the pullback of H_{fluids} through the Poisson map $\mathcal{J}_1$, so that we can carry out the reduction described in section **2.5.1**.

Unfortunately, this exact reduction is not possible. The extent to which it fails is quantified by the deviation of the distribution function f from its associated *local Maxwellian* f_m, which is defined as

$$f_m(x, p) = \frac{\rho}{(2\pi\theta)^{n/2}} \exp\left(-\frac{|p - u|^2}{2\theta} \right). \tag{4.4.5}$$

The local Maxwellian f_m is so constructed to have the same mass density, mean velocity and kinetic-theory temperature as f. The dependence of f_m on f is highly nonlinear. Substituting f_m into (4.4.1c) and rearranging gives

$$\theta[f] = \frac{\rho[f]^{2/n}}{2\pi\mathrm{e}} \exp\left(-\frac{2}{n} \frac{s[f_m]}{\rho[f]} \right), \tag{4.4.6}$$

where $\mathrm{e} = \exp(1)$. On the other hand, choosing $C = -(n/2)\log(2\pi\mathrm{e})$ in (4.4.3) and rearranging gives

$$T(\rho[f], s[f]) = \frac{\rho[f]^{2/n}}{2\pi\mathrm{e}} \exp\left(-\frac{2}{n}\frac{s[f]}{\rho[f]}\right). \tag{4.4.7}$$

The expressions (4.4.6) and (4.4.7) are remarkably similar, with the only difference being that $s[f]$ appears in (4.4.6) while $s[f_m]$ appears in (4.4.7). This difference can also be expressed in terms of the relative entropy density of f against f_m. We define the *relative entropy density* of f_1 against f_2 as [32, 150]

$$r[f_1|f_2] = \int d^n p \ \left(f_1 \log(f_1/f_2) + f_1 - f_2\right), \tag{4.4.8}$$

where f_1 and f_2 are positive distribution functions. Here $r[f_1|f_2]$ is a non-negative function of x, with equality at fixed x_0 if and only if $f_1(x_0, p) = f_2(x_0, p)$. We can show that $s[f] - s[f_m] = r[f|f_m]$ using properties of the local Maxwellian [150], so

$$\theta[f] = T\left(\rho[f], s[f_m]\right) = T\left(\rho[f], s[f]\right) \exp\left(\frac{2}{n}\frac{r[f|f_m]}{\rho[f]}\right). \tag{4.4.9}$$

From the non-negativity of $r[f|f_m]$ and (4.4.9), we see that $\theta[f] \geq T(\rho[f], s[f])$ with equality if and only if $f = f_m$. Putting everything together, we have:

Proposition 4.3. *The kinetic-theory Hamiltonian $H_{KT}[f]$ from (4.4.2), defined on the space $C^\infty(T^*M)_+$ of positive 1-particle distribution functions, is related to the fluid Hamiltonian $H_{fluids}[m, \rho, s]$ from (4.4.4), defined on the space $\mathfrak{s}_1^*$ of hydrodynamic variables for an ideal compressible fluid with non-constant entropy by*

$$H_{KT} = \mathcal{J}_1^* H_{fluids} + \Delta H, \tag{4.4.10}$$

where $\mathcal{J}_1 : C^\infty(T^*M)_+ \to \mathfrak{s}_1^*$ is the Poisson map described in (4.3.1) with $A = 1$, and

$$\Delta H[f] = \frac{n}{2} \int d^n x \ \rho[f]\theta[f] \left(1 - \exp\left(-\frac{2}{n}\frac{r[f|f_m]}{\rho[f]}\right)\right). \tag{4.4.11}$$

This functional satisfies the inequality $\Delta H[f] \geq 0$, with equality if and only if the distribution function f is a local Maxwellian everywhere, i.e. $f(x, p) = f_m(x, p)$.

A similar result holds for the Vlasov–Poisson equation. The extra mean-field potential in the Hamiltonian functional $H_{VP}[f]$ (4.2.14) depends on $\rho[f]$ only, so it also factors through the Poisson map $\mathcal{J}_1$. If we ignore the relative entropy of the distribution function against its local Maxwellian, the Vlasov–Poisson system reduces to the Euler–Poisson equations [48, 197], with non-constant entropy.

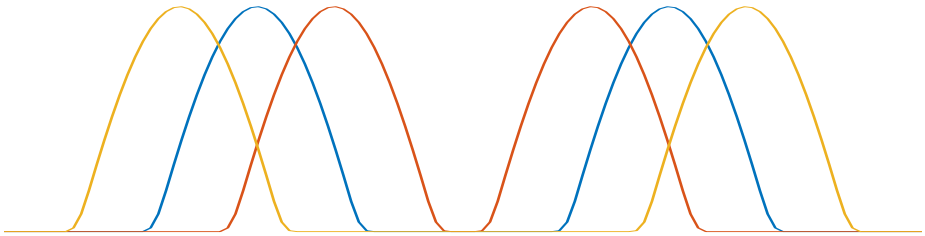


Figure 4.1: Two-bump functions $f_c(p) = (B(p-c) + B(p+c))/2$ for various c.

Corollary 4.1. *The Vlasov–Poisson Hamiltonian $H_{VP}[f]$ from (4.2.14) can be written as*

$$H_{VP} = \mathcal{J}_1^* \left(H_{fluids} + H_{static}\right) + \Delta H, \tag{4.4.12}$$

where $H_{fluids}[m, \rho, s]$ is the fluid Hamiltonian (4.4.4) for an uncharged monatomic ideal gas, ΔH is as in (4.4.11), and $H_{static}[\rho]$ is the electrostatic energy of a charged fluid, defined by

$$H_{static}[\rho] = \int d^n x \, \frac{e\rho\varphi[\rho]}{2}, \tag{4.4.13}$$

where the electric potential φ is related to the charge density $e\rho$ by Poisson's equation (4.2.15).

An entirely analogous result holds for a self-gravitating system as well, since the potential energy in the self-gravitating Hamiltonian $H_{SG}[f]$ (4.2.16) is exactly that of $H_{VP}[f]$ with the replacement $e^2 \mapsto -\mathrm{G}$. In this case ignoring the relative entropy reduces the Jeans equation to the Euler–Poisson equations under the same replacement.

Remark 4.1. We cannot reduce the kinetic theory description for an ideal gas to a hydrodynamic description exactly, even if we include the entropy density using the Poisson map $\mathcal{J}_1$. Suppose that we are given an unknown distribution function f, and that we know the values of the integrals $m[f] = \int d^n p \, pf$ and $\int d^n p \, y(f)$ for all real functions y. From this information alone, we cannot determine the kinetic-theory temperature $\theta[f]$ in general. At a fixed x, if we rearrange the p-space $T_x M$ in a volume-preserving way, the values of the integrals $\int d^n p \, y(f)$ remain unchanged. However, there are examples of such volume-preserving rearrangements where $m[f]$ remains unchanged while $\theta[f]$ changes. Indeed, consider the one-dimensional example $f_c(p) = (B(p-c) + B(p+c))/2$, where $B(x)$ is a bump function with support in $[-1/2, 1/2]$; see figure 4.1. For all $c \geq 1$, the integrals $\int dp \, y(f_c)$ for any given real function y coincide, yet $\theta[f_c]$ can be made arbitrary large as c increases. We conclude that $\theta[f]$, and hence $H_{KT}[f]$, cannot be determined from the image $\mathsf{J}[f]$ (4.3.2) of f under the Poisson map J (4.3.23), and in particular any of the $\mathcal{J}_A$. This is yet another instance of the *moment closure problem* in kinetic theory, where an exact description of a kinetic system using a finite number of hydrodynamic variables is impossible in general.

The upside to Proposition 4.3 is that, if we neglect the term ΔH in the kinetic-theory Hamiltonian H_{KT} (4.4.10) by ignoring the relative entropy density $r[f|f_m]$, the remaining nonlinear functional is precisely the pullback of the fluid Hamiltonian H_{fluids} through the Poisson map $\mathcal{J}_1$. For small deviations from a local Maxwellian $f = f_m(1 + \epsilon h)$, the relative entropy density $r[f|f_m]$ and hence the term ΔH are formally $O(\epsilon^2)$, so $\mathcal{J}_1^* H_{fluids}$ can be thought of as a truncation of H_{KT} in the limit $\epsilon \to 0$. This approximation gives a manifestly Hamiltonian derivation of the compressible Euler equations, endowing them with a Hamiltonian structure that is inherited from kinetic theory through $\mathcal{J}_1$. Neglecting ΔH (4.4.11) in H_{KT} or H_{VP} is thus an improvement on the ansatz suggested in (4.2.23) as we can relate it to the local Maxwellian assumption $f \simeq f_m$.

This should be compared to the usual derivation of hydrodynamics from kinetic theory, where the full Boltzmann equation in the strongly collisional limit $\mathrm{Kn} \to 0$ is considered instead of the collisionless Boltzmann equation. At leading order, the distribution function is constrained to be local Maxwellian, and taking moments results in compressible Euler equations; cf. the Chapman–Enskog expansion studied in section **1.1**. The Chapman–Enskog expansion offers a formal asymptotic derivation of hydrodynamics as an approximation to kinetic theory in the strongly collisional limit, but it does not explain why the compressible Euler equations are Hamiltonian. Conversely, Proposition 4.3 addresses the Hamiltonian structure of the compressible Euler equations, but has no bearing on their validity as an asymptotic limit of kinetic theory. Similarly, we can obtain a "naive fluid model" for an electrostatic plasma by ignoring ΔH in $H_{VP}[f]$, and likewise for a self-gravitating system. Corollary 4.1 suggests that the naive fluid models obtained this way inherit the Hamiltonian structure of 1-particle kinetic theory through the Poisson map $\mathcal{J}_1$, but it has no bearing on the physical validity of such models.

For the rest of the section, we study the properties of ΔH (4.4.11). In section **4.4.1** we consider bounds on ΔH in the near global Maxwellian regime, and in section **4.4.2** we consider improved approximations to ΔH for isotropic near local Maxwellian distribution functions.

4.4.1 ΔH in the near global Maxwellian regime

In this section we show that the term ΔH in (4.4.10) stays small uniformly in time if the initial distribution function f is sufficiently close to a *global Maxwellian*, in a sense made precise by the relative entropy. This is not a proof that the solutions of the collisionless Boltzmann equation approximates the solutions of the compressible Euler equations.

In the following we work exclusively on $\mathbb{T}^n$. This choice is motivated by the need to define the quantities

$$\rho_0 = \frac{1}{\mathrm{vol}\,(\mathbb{T}^n)} \int dV\ f(x,p), \tag{4.4.14a}$$

$$\rho_0 u_0 = \frac{1}{\mathrm{vol}\,(\mathbb{T}^n)} \int dV\ pf(x,p), \tag{4.4.14b}$$

$$\rho_0 \left(|u_0|^2 + n\theta_0\right) = \frac{1}{\mathrm{vol}\,(\mathbb{T}^n)} \int dV\ |p|^2 f(x,p), \tag{4.4.14c}$$

$$f_M(x,p) = \frac{\rho_0}{(2\pi\theta_0)^{n/2}} \exp\left(-\frac{|p-u_0|^2}{2\theta_0}\right). \tag{4.4.14d}$$

Here ρ_0 is the mean mass density, u_0 is the mean velocity, and θ_0 is the mean temperature. The function f_M is the *global Maxwellian* with the same mean mass density, mean velocity and mean temperature as f. The mean mass density is only defined on manifolds with finite volume, and there is no straightforward interpretation of the mean velocity on manifolds that are not domains in $\mathbb{R}^n$ or $\mathbb{T}^n$, so $\mathbb{T}^n$ is simplest choice of a connected manifold without boundary on which the global Maxwellian is unambiguously defined.

The mean mass density ρ_0 is a Casimir functional of the kinetic-theory Poisson bracket (2.6.43). The mean velocity u_0 and mean temperature θ_0 are constants of motion because they Poisson commute with H_{KT} (4.4.2).

We define the total *relative entropy* of f_1 against f_2, where f_1 and f_2 are (positive) distribution functions as the x-integral of the relative entropy density $r[f_1|f_2]$ (4.4.8):

$$R[f_1|f_2] = \int dV\ \left(f_1 \log(f_1/f_2) + f_1 - f_2\right). \tag{4.4.15}$$

This quantity is non-negative and is zero if and only if $f_1 = f_2$. The relative entropy $\mathcal{R}_{in}$ of f against its associated global Maxwellian

$$\mathcal{R}_{in} = R[f|f_M] = \int dV\ f \log f - \int dV\ f \log f_M. \tag{4.4.16}$$

is a constant of motion, since the first term is a Casimir functional of the kinetic theory bracket, and the second term is a constant of motion. Now we state the main result of this section:

Proposition 4.4. *Let $\Delta H[f]$ be as in (4.4.10). Suppose that f evolves according to the collisionless Boltzmann equation. Then the following inequality holds:*

$$\Delta H[f] \leq 2\theta_0 \mathcal{R}_{in}, \tag{4.4.17}$$

where the right-hand side consists only of constants of motion.

Proof. To avoid notational clutter, we suppress the f-dependence from functionals of f except for the relative entropies. We would like to bound the term

$$\Delta H = \frac{n}{2} \int d^n x \, \rho\theta \left(1 - \exp\left(-\frac{2}{n}\frac{r[f|f_m]}{\rho}\right)\right), \tag{4.4.18}$$

which contains the product of the temperature with an entropy-like term. This can be done using the physical a priori estimates in [150], chapter 3.1. First note that

$$\mathcal{R}_{in} = R[f|f_M] = R[f|f_m] + R[f_m|f_M]. \tag{4.4.19}$$

The first term is the relative entropy of f against its local Maxwellian f_m, and the second term is the relative entropy of the local Maxwellian f_m against the global Maxwellian f_M. Both quantities are manifestly non-negative. To simplify notation, we write $\mathcal{R}_m = R[f|f_m]$ and $\mathcal{R}_M = R[f_m|f_M]$.

1. First we study the entropy-like term $\eta = 1 - \exp\left(-2r[f|f_m]/n\rho\right)$. From the elementary inequality $0 \leq 1 - \exp(-x) \leq \min(1, x)$ for $x \geq 0$, we have

   $$0 \leq \eta \leq 1, \quad \text{and} \int d^n x \, \rho\eta \leq \frac{2}{n}\mathcal{R}_m. \tag{4.4.20}$$

   We can combine these inequalities to obtain control over any power of η in terms of the relative entropy:

   $$\int d^n x \, \rho\eta^a \leq \frac{2}{n}\mathcal{R}_m \quad \text{for all } a \in \mathbb{Z}^+, \tag{4.4.21}$$

   so the Cauchy–Schwartz and Hölder inequalities are effective in controlling products of η with other entropy-bounded terms.

2. We move on to the thermal term. A direct computation shows that

   $$\mathcal{R}_M = \int d^n x \, \left(\rho_0 h\left(\frac{\rho - \rho_0}{\rho_0}\right) + \frac{n}{2}\rho k\left(\frac{\theta - \theta_0}{\theta_0}\right) + \rho\frac{|u - u_0|^2}{2\theta_0}\right), \tag{4.4.22}$$

   where $h(z) = (1+z)\log(1+z) - z$ and $k(z) = z - \log(1+z)$. Both h and k are non-negative convex functions that are locally quadratic for small z, but subquadratic for $z \gg 1$. For infinitesimal fluctuations $\mathcal{R}_M$ behaves like an L^2-type norm, but for finite fluctuations, control on the relative entropy typically only implies control on the L^1-size of the fluctuations (e.g. by an argument in [32], p.20). Nonetheless, by considering *renormalised fluctuations* ([150], p.52), we can obtain a sharper result that is sufficient for our purposes. Define the *renormalised thermal fluctuation* $\hat{\theta}$ by

   $$\hat{\theta} = \sqrt{\frac{\theta}{\theta_0}} - 1, \quad \text{so } \frac{\theta - \theta_0}{\theta_0} = 2\hat{\theta} + \hat{\theta}^2. \tag{4.4.23}$$

Then the elementary inequality $k(z) \geq (\sqrt{1+z}-1)^2$ implies that

$$\int d^n x\ \rho\hat{\theta}^2 \leq \int d^n x\ \rho k\left(\frac{\theta-\theta_0}{\theta_0}\right) \leq \frac{2}{n}\mathcal{R}_M, \tag{4.4.24}$$

so the renormalised thermal fluctuation $\hat{\theta}$ is L^2-controlled. While this only implies L^1-control on the true thermal fluctuation $(\theta-\theta_0)/\theta_0$, the decomposition (4.4.23) gives us a handle on the products of $(\theta-\theta_0)$ with other entropy-bounded terms, in particular η.

Now we are ready to derive a bound for ΔH. We decompose

$$\Delta H = \frac{n}{2}\int d^n x\ \rho\theta\eta = \theta_0\left(\frac{n}{2}\int d^n x\ \rho\eta + \frac{n}{2}\int d^n x\ \rho\frac{\theta-\theta_0}{\theta_0}\eta\right). \tag{4.4.25}$$

The first term in the brackets is bounded by $\mathcal{R}_m$ by (4.4.20). To bound the second term,

$$\begin{aligned}
\frac{n}{2}\int d^n x\ \rho\frac{\theta-\theta_0}{\theta_0}\eta &= \frac{n}{2}\int d^n x\ \rho\left(2\hat{\theta}+\hat{\theta}^2\right)\eta \\
&= n\int d^n x\ \rho\hat{\theta}\eta + \frac{n}{2}\int d^n x\ \rho\hat{\theta}^2\eta, \\
&\leq n\left(\int d^n x\rho\hat{\theta}^2\right)^{1/2}\left(\int d^n x\rho\eta^2\right)^{1/2} + \frac{n}{2}\int d^n x\ \rho\hat{\theta}^2, \\
&\leq n\left(\frac{2}{n}\mathcal{R}_M\right)^{1/2}\left(\frac{2}{n}\mathcal{R}_m\right)^{1/2} + \mathcal{R}_M \\
&\leq \mathcal{R}_M + \mathcal{R}_m + \mathcal{R}_M.
\end{aligned} \tag{4.4.26}$$

Thus $\Delta H \leq \theta_0(2\mathcal{R}_M + 2\mathcal{R}_m) = 2\theta_0\mathcal{R}_{in}$, which is precisely the claimed inequality (4.4.17). □

The inequality (4.4.17) is effective as $\mathcal{R}_{in} \to 0$. In this limit, the Mach number of the gas is necessarily small, since

$$\int d^n x\ \rho\frac{|u-u_0|^2}{2\theta_0} \leq \mathcal{R}_{in}, \tag{4.4.27}$$

by (4.4.22).

The inequality (4.4.17) holds regardless of how f evolves. However, if f does not evolve according to the collisionless Boltzmann equation, the right-hand side of (4.4.17) is not necessarily a constant of motion. Nonetheless, if f evolves according to the *Vlasov–Poisson equation* (see section **2.6.3**), a statement similar to Proposition 4.4 holds. We show this by finding constants of motion of the Vlasov–Poisson equation that bound θ_0 and $\mathcal{R}_{in}$ from above.

Define the modified temperature Φ_0 by

$$\rho_0 \left(|u_0|^2 + n\Phi_0 \right) \mathrm{vol}\,(\mathbb{T}^n) = \int dV\ |p|^2 f(x,p) + e^2 \int d^n x d^n x' \rho(x)\rho(x') G(x,x'). \tag{4.4.28}$$

The right-hand side is $2H_{VP}[f]$ (2.6.50), which is a constant of motion of the Vlasov–Poisson equation. Since ρ_0 and u_0 are constants of motion of the Vlasov–Poisson equation as well, so is Φ_0. The integral operator with kernel $G(x,x')$ is positive semidefinite, so comparing (4.4.14c) and (4.4.28) gives $\theta_0 \leq \Phi_0$.

We then seek a constant of motion $\mathcal{S}_{in}$ that bounds $\mathcal{R}_{in}$ from above. The explicit expression for $\mathcal{R}_{in}$ (4.4.16) is

$$\mathcal{R}_{in} = \int dV\ f \log f + \rho_0 \mathrm{vol}\,(\mathbb{T}^n) \left(-\log \rho_0 + \frac{n}{2} \log \theta_0 + \frac{n}{2} \log (2\pi \mathrm{e}) \right). \tag{4.4.29}$$

Since $\log \theta_0 \leq \log \Phi_0$, choosing

$$\mathcal{S}_{in} = \int dV\ f \log f + \rho_0 \mathrm{vol}\,(\mathbb{T}^n) \left(-\log \rho_0 + \frac{n}{2} \log \Phi_0 + \frac{n}{2} \log (2\pi \mathrm{e}) \right) \tag{4.4.30}$$

gives an upper bound for $\mathcal{R}_{in}$ by constants of motion.

Corollary 4.2. *Let $\Delta H[f]$ be as in (4.4.10). Suppose that f evolves according to the Vlasov–Poisson equation. Then the following inequality holds:*

$$\Delta H[f] \leq 2\Phi_0 \mathcal{S}_{in}, \tag{4.4.31}$$

where the right-hand side consists only of constants of motion.

A similar statement for the *Jeans equation* of a self-gravitating system does not hold however, since the potential energy in the self-gravitating Hamiltonian $H_{SG}[f]$ (2.6.53) has the opposite sign. While the inequality (4.4.17) still holds, we cannot find an upper bound for θ_0 in terms of constants of motion by the same method due to the sign difference.

4.4.2 Approximate reduction for isotropic near local Maxwellian distribution functions

In this section we develop an approximation of $\Delta H[f]$ (4.4.11) for *isotropic* near local Maxwellian distribution functions in terms of the generalised entropy variables $s_a[f]$ constructed in section **4.3**. Using this procedure, we obtain Hamiltonians of the form

$$H_A[\rho, s_1, \ldots, s_A] = \int d^n x \left(\frac{|m|^2}{2\rho} + \frac{n}{2} \rho \tilde{T}(\rho, s_1, \ldots, s_A) \right), \quad A \geq 2, \tag{4.4.32}$$

which generates the compressible Euler equations (2.6.1a, 2.6.1b), with the entropy equation (2.6.1c) for each generalised entropy s_a. The pressure P is given by

$$P(\rho, s_1, \ldots, s_A) = \frac{n}{2}\left(\rho\frac{\partial(\rho\tilde{T})}{\partial\rho} + \sum_{a=1}^{A} s_a \frac{\partial(\rho\tilde{T})}{\partial s_a} - \rho\tilde{T}(\rho, s_1, \ldots, s_A)\right). \tag{4.4.33}$$

These hydrodynamic Hamiltonian systems on $\mathfrak{s}_A^*$ are approximate reductions of kinetic theory in a sense similar to Proposition 4.3, namely that

$$H_{KT} = \mathcal{J}_A^* H_A + (\Delta H - \Delta H_A) \tag{4.4.34}$$

holds, with ΔH_A being an approximation of ΔH. This improves on the approximation of dropping ΔH entirely in the case $A = 1$ at the cost of introducing extra generalised entropy variables, which does not necessarily have a clear physical interpretation.

Let $f = f_m(1 + \epsilon h)$, where f_m is the local Maxwellian associated to f (4.4.5), and ϵ be a small parameter. In what follows, we will consider a formal perturbation expansion in ϵ. The relative entropy density (4.4.8) of f against f_m is then

$$r[f|f_m] = \frac{\epsilon^2}{2}\int d^n p\; f_m h^2 + O(\epsilon^3). \tag{4.4.35}$$

Substituting (4.4.35) in (4.4.9) gives $\theta - T = O(\epsilon^2)$, whence

$$\Delta H = \frac{\epsilon^2}{2}\int dV\; \theta f_m h^2 + O(\epsilon^3) = \frac{\epsilon^2}{2}\int dV\; T f_m h^2 + O(\epsilon^3), \tag{4.4.36}$$

so ΔH behaves like a weighted L^2-norm on the non-Maxwellian deviation h in the near local Maxwellian limit $\epsilon \to 0$. An approximate reduction becomes possible if we can express $\int d^n p f_m h^2$ in terms of hydrodynamic variables to leading order in ϵ. This can be achieved when h is *isotropic* in p, namely that

$$h(x, p) = h(x, \chi), \quad \text{where } \chi = \frac{|p - u|^2}{2\theta}. \tag{4.4.37}$$

The assumption that f is isotropic is known as the *Eddington approximation* in the kinetic theory of radiative transfer [4, 111, 180]. For any isotropic function g, we have

$$\int d^n p\; f_m g = \rho\int_0^\infty d\chi\; F_n g, \quad \text{where } F_n(\chi) = \frac{1}{\Gamma(n/2)}\chi^{(n/2)-1}\mathrm{e}^{-\chi}. \tag{4.4.38}$$

Let us also expand h in terms of *Laguerre polynomials* [5] (see appendix **C**):

$$h(x, \chi) = \sum_{b=2}^{\infty} \beta_b(x) L_b^{(n/2)-1}(\chi), \tag{4.4.39}$$

where the $b = 0$ and $b = 1$ terms are dropped because f is required to have the same 1 and χ moments as f_m. The expression of ΔH in terms of the β_b is

$$\Delta H = \frac{\epsilon^2}{2} \int d^n x \, \rho T \sum_{b=2}^{\infty} \frac{\Gamma(b + n/2)}{\Gamma(b+1)\Gamma(n/2)} \beta_b^2 + O(\epsilon^3). \tag{4.4.40}$$

In the following we show that the β_b can be expressed solely in terms of the density ρ and the generalised entropy densities (4.3.2) $s_1, s_2, \ldots s_b$ to leading order in ϵ, namely that

$$\beta_b = \frac{1}{\epsilon} \tilde{\beta}_b(\rho, s_1, s_2, \ldots, s_b) + O(\epsilon), \tag{4.4.41}$$

which permits ΔH (4.4.40) to be approximated by hydrodynamic variables with $O(\epsilon^3)$ error. The $\tilde{\beta}_b$ are $O(\epsilon)$ quantities formed by differences of nominally $O(1)$ quantities and have no explicit ϵ-dependence, as we shall see.

For notational simplicity, we write $\eta_a = s_a/\rho$ for $a \geq 1$. From (4.3.2) we have

$$\begin{aligned}
\eta_a =& \frac{1}{\rho} \int d^n p \, f (\log f)^a = \int d^n p \, \frac{f_m}{\rho} (1 + \epsilon h) \left(\log f_m + \log(1 + \epsilon h) \right)^a, \\
=& \int_0^\infty d\chi \, F_n \left(\log \left(\frac{\rho}{(2\pi\theta)^{n/2}} \right) - \chi \right)^a \\
&+ \epsilon \int_0^\infty d\chi \, F_n h \left(\log \left(\frac{\rho}{(2\pi\theta)^{n/2}} \right) - \chi \right)^{a-1} \left(\log \left(\frac{\rho}{(2\pi\theta)^{n/2}} \right) + a - \chi \right) + O(\epsilon^2).
\end{aligned} \tag{4.4.42}$$

The $O(1)$ term in the expression (4.4.42) for η_a is the value of η_a when f is a local Maxwellian, which we denote as $\bar{\eta}_a$. The $O(\epsilon)$ term in (4.4.42) linear in the coefficients $\beta_2, \ldots \beta_a$ in h by the properties of the Laguerre polynomials. From the $a = 1$ case of (4.4.42) we find

$$\log \left(\frac{\rho}{(2\pi\theta)^{n/2}} \right) = \eta_1 + \frac{n}{2} - \frac{r[f|f_m]}{\rho} = \eta_1 + \frac{n}{2} + O(\epsilon^2), \tag{4.4.43}$$

so we can rewrite (4.4.42) for $a \geq 2$ as a linear system of equations

$$\eta_a - \bar{\eta}_a(\eta_1) = \epsilon \sum_{b=2}^{\infty} M(\eta_1)_{ab} \beta_b + O(\epsilon^2), \tag{4.4.44}$$

where M_{ab} is a lower triangular matrix with non-zero diagonal entries. The left-hand side $\eta_a - \bar{\eta}_a(\eta_1)$ of (4.4.44) is an $O(\epsilon)$ quantity that is the difference of two nominally $O(1)$ quantities. The solution to (4.4.44) is

$$\beta_b = \frac{1}{\epsilon} \sum_{c=2}^{\infty} (M^{-1})(\eta_1)_{bc} \left(\eta_c - \bar{\eta}_c(\eta_1) \right) + O(\epsilon), \tag{4.4.45}$$

where M^{-1}_{bc}, the inverse matrix of M_{ab}, is again lower triangular with non-zero diagonal entries[6]. This gives a solution of the form (4.4.41). The explicit expressions for $\bar{\eta}_a, M(\eta_1)_{ab}, \tilde{\beta}_a$ up to order 4 are detailed in appendix **C**.

Returning to the problem of approximating ΔH, consider for $A \geq 2$ the quantities

$$\Delta H_A[f] = \frac{1}{2}\int d^n x \rho[f] T(\rho[f], s_1[f]) \sum_{b=2}^{A} \frac{\Gamma(b+n/2)}{\Gamma(b+1)\Gamma(n/2)} \bar{\beta}_b(\rho, s_1, s_2, \ldots, s_b)^2, \tag{4.4.46}$$

and let $\Delta H_\infty = \lim_{A\to\infty} \Delta H_A$. We know from (4.4.40) that $\Delta H - \Delta H_\infty = O(\epsilon^3)$. Each ΔH_A factors through the Poisson map $\mathcal{J}_A : C^\infty(T^*M)_+ \to \mathfrak{s}_A^*$ (4.3.1). The infinite sum ΔH_∞ does not factor through $\mathcal{J}_A$ for any finite A, but it factors through the larger Poisson map $\mathsf{J} : C^\infty(T^*M)_+ \to \mathrm{Vect}(M)^* \times P\Omega^n(M)$ (4.3.23), since the Tsallis entropy density $\rho_\xi[f]$ (4.3.24) is the generating function for all the generalised entropy densities $s_a[f]$.

The use of ΔH_A instead of the full series ΔH_∞ corresponds to truncating the Laguerre polynomial expansion of h (4.4.39) at order A

$$h(x,\chi) = \sum_{b=2}^{A} \beta_b(x) L_b^{(n/2)-1}(\chi), \tag{4.4.47}$$

so hydrodynamic models formed with the Hamiltonian
$H_A = H_{fluids}[m,\rho,s_1] + \Delta H_A[\rho, s_1, \ldots, s_A]$ on $\mathfrak{s}_A^*$ can be considered as a finite isotropic moment truncation for the non-Maxwellian deviation h in the near local Maxwellian limit $\epsilon \to 0$. For example, the Hamiltonian H_2 on $\mathfrak{s}_2^*$ is (using (C.0.5a))

$$H_2[m,\rho,s_1,s_2] = \int d^n x \left(\frac{|m|^2}{2\rho} + \frac{n}{2}\rho T(\rho, s_1)\left(1 + \frac{(2s_2 - 2s_1^2 - n\rho)^2}{2n^2(n+2)\rho^2}\right)\right), \tag{4.4.48}$$

where T is as in (4.4.7).

Remark 4.2. The isotropic assumption of h is itself a truncation of the full tensor Hermite polynomial expansion of h by discarding the non-isotropic moments [4, 111, 180]. While the relationship (4.4.36) between ΔH and h holds in the near local Maxwellian regime regardless of whether h is isotropic, we cannot obtain the contribution from the non-isotropic parts of h to ΔH using the generalised entropies. The non-isotropic part of h does not enter the $O(\epsilon)$ part of (4.4.42) because $\log f_m$ is an isotropic function. If one attempts to continue the expansion $h = h^{(0)} + \epsilon h^{(1)} + \ldots$, the $O(\epsilon^2)$ part of (4.4.42) gives an unclosed

[6]For any $k \times k$ lower-triangular matrix M with inverse M^{-1}, the inverse of the top-left $q \times q$ submatrix of M coincides with the top-left $q \times q$ submatrix of M^{-1}, a property easily proven by induction. In practice this means that the infinite sum in (4.4.45) can be truncated at $c = b$, and the entries of M^{-1} up to this order can be calculated by inverting a top-left square submatrix of M of appropriate size.

relationship between the isotropic part of $h^{(1)}$ and the non-isotropic part of $h^{(0)}$, both of which are unknown. Therefore, our calculations only lead to closed expressions if we assume $h^{(0)}$ has no non-isotropic part i.e. h is isotropic to leading order in ϵ.

4.5 Hydrodynamic reductions using singular Poisson submanifolds

We can also construct a hydrodynamic reduction of kinetic theory by seeking a Poisson map from a space of hydrodynamic variables *into* the space of kinetic distribution functions. These reductions are always exact since the kinetic-theory Hamiltonian can always be pulled back to the hydrodynamic space, but they correspond only to special configurations in the image of the Poisson map. These maps are often *singular*, in the sense that they do not result in smooth distribution functions f. However, these singularities can often be mollified by integrating out the p-dependence, which leads to Poisson maps into the space $\mathfrak{S}^*$ of p-moments.

4.5.1 Cold plasma reduction

In this section we discuss *cold plasma reduction* [70, 72, 73, 176, 177], corresponding to an ansatz of the form

$$f(x,p,t) = \rho(x,t)\delta^n(p-u(x,t)), \tag{4.5.1}$$

where ρ is the mass density and $u = m/\rho$ is the 1-form representing the local velocity. The ansatz (4.5.1) is called the *cold plasma approximation* or *cold beam approximation* because the kinetic-theory temperature $\theta[f]$ (4.4.14c) is zero. The ansatz (4.5.1) can be considered as a map from $(u,\rho) \in \mathfrak{s}^*_{0u}$ to the space of distribution functions. However, the image is a singular distribution localised on the section $u : M \to T^*M$. We can work around this singularity by instead proposing a map from $\mathfrak{s}^*_{0u}$ to the space of moments $\mathfrak{S}^*$. The moments of such f are

$$A^{(a)}[f]_{i_1\dots i_a} = \int d^n p\, p_{i_1}\dots p_{i_a} f = \rho u_{i_1}\dots u_{i_a}. \tag{4.5.2}$$

This motivates the following construction:

Proposition 4.5. *The map $\mathcal{J}_{cold} : \mathfrak{s}^*_{0u} \to \mathfrak{S}^*$, defined by*

$$\mathcal{J}_{cold} : (u,\rho) \mapsto \left(A^{(0)}, A^{(1)}, \dots\right), \quad A^{(a)}{}_{i_1\dots i_a} = \rho u_{i_1}\dots u_{i_a} \tag{4.5.3}$$

is a Poisson map with respect to the bracket (2.6.10) on $\mathfrak{s}^*_{0u}$ and the Kuperschmidt–Manin bracket (4.5.7) on $\mathfrak{S}^*$.

Proof. Let $F = \tilde{F} \circ \mathcal{I}_{cold}$ and $G = \tilde{G} \circ \mathcal{I}_{cold}$. By the functional chain rule we have

$$\frac{\delta F}{\delta \rho} = \sum_{a=0}^{\infty} \frac{\delta \tilde{F}}{\delta A^{(a)}{}_{i_1 \dots i_a}} u_{i_1} \dots u_{i_a}, \tag{4.5.4a}$$

$$\frac{\delta F}{\delta u_k} = \sum_{a=0}^{\infty} a \frac{\delta \tilde{F}}{\delta A^{(a)}{}_{i_1 \dots i_{a-1} k}} \rho u_{i_1} \dots u_{i_{a-1}}, \tag{4.5.4b}$$

where the $a = 0$ term in (4.5.4b) can be taken as 0 since it is multiplied to 0, so the ill-defined tensor "$\otimes^{-1} u$" is not a problem. We have

$$\begin{aligned}
&\{F, G\}_{\mathfrak{s}^*_{0u}} \\
&= -\sum_{a,b=0}^{\infty} \int d^n x \, \rho \Bigg(-ab \frac{\delta \tilde{F}}{\delta A^{(a)}{}_{i_1 \dots i_{a-1} l}} u_{i_1} \dots u_{i_{a-1}} \frac{\delta \tilde{G}}{\delta A^{(b)}{}_{j_1 \dots j_{b-1} k}} u_{j_1} \dots u_{j_{b-1}} \nabla_l u_k \\
&\qquad\qquad + a \frac{\delta \tilde{F}}{\delta A^{(a)}{}_{i_1 \dots i_{a-1} l}} u_{i_1} \dots u_{i_{a-1}} \nabla_l \left(\frac{\delta \tilde{G}}{\delta A^{(b)}{}_{j_1 \dots j_b}} u_{j_1} \dots u_{j_b} \right) \Bigg) \\
&\quad - (F \leftrightarrow G) \\
&= -\sum_{a,b=0}^{\infty} \int d^n x \, \rho u_{i_1} \dots u_{i_{a-1}} u_{j_1} \dots u_{j_{b-1}} u_k a \frac{\delta \tilde{F}}{\delta A^{(a)}{}_{i_1 \dots i_{a-1} l}} \nabla_l \frac{\delta \tilde{G}}{\delta A^{(b)}{}_{j_1 \dots j_{b-1} k}} \\
&\quad - (F \leftrightarrow G) \\
&= -\sum_{a,b=0}^{\infty} \left\langle A^{(a+b-1)}[u, \rho], \left[\frac{\delta \tilde{F}}{\delta A^{(a)}}, \frac{\delta \tilde{G}}{\delta A^{(b)}} \right] \right\rangle_{\mathfrak{S}_{a+b-1}} = \{\tilde{F}, \tilde{G}\}_{KM} \circ \mathcal{I}_{cold},
\end{aligned} \tag{4.5.5}$$

where we recognise the term in the second-to-last line (4.5.5) to be one half of the symmetric Schouten bracket (4.2.5). Thus $\mathcal{I}_{cold}$ is a Poisson map. □

In particular, the Vlasov–Poisson Hamiltonian (4.2.14) can be pulled back to $\mathfrak{s}^*_{0u}$ through the map $\mathcal{I}_{cold}$, which gives a reduced Hamiltonian system on $\mathfrak{s}^*_{0u}$ for the dynamics of a cold electrostatic plasma. Interestingly, this results in the same Hamiltonian system if we take an approximate reduction using the Poisson map $\mathfrak{S}^* \to \mathfrak{S}^*_0 \oplus \mathfrak{S}^*_1 = \mathfrak{s}^*_0$ by making the uncontrolled approximation $A^{(2)} = A^{(1)} \otimes A^{(1)} / A^{(0)}$ directly in the Hamiltonian (4.2.14).

4.5.2 Waterbag reduction in one dimension

In this section we discuss *waterbag reduction* in one dimension, corresponding to piecewise-constant distribution functions known as *waterbag distribution functions* [144, 195] and is closely related to the Benney hydrodynamic chain [15]. For this section we consider the case $M = \mathbb{R}$ only; some extensions of the techniques in this section to two dimensions have

been considered in [39]. In this one-dimensional setting, the moments

$$A^{(k)} = \int dp\, p^k f \tag{4.5.6}$$

are simply functions on $\mathbb{R}$. The Kuperschmidt–Manin bracket (4.2.9) on the space of moments $\mathfrak{S}^*(\mathbb{R})$ simplifies to

$$\begin{aligned}\{F,G\}_{KM} &= -\int dx\, \sum_{k,l=0}^{\infty} \frac{\delta F}{\delta A^{(k)}} \left((k+l) A^{(k+l-1)} \frac{\partial}{\partial x} \frac{\delta G}{\delta A^{(l)}} + l \frac{\delta G}{\delta A^{(l)}} \frac{\partial A^{(k+l-1)}}{\partial x} \right), \\ &= -\int dx\, \sum_{k,l=0}^{\infty} A^{(k+l-1)} \left(k \frac{\delta F}{\delta A^{(k)}} \frac{\partial}{\partial x} \frac{\delta G}{\delta A^{(l)}} - l \frac{\delta G}{\delta A^{(l)}} \frac{\partial}{\partial x} \frac{\delta F}{\delta A^{(k)}} \right). \end{aligned} \tag{4.5.7}$$

In the following we construct a Poisson map into $\mathfrak{S}^*(\mathbb{R})$.

Consider the space $\mathfrak{A}_N$ of N-tuples of *waterbag variables* $a^{(1)}(x), \ldots, a^{(N)}(x)$, with each $a^{(n)} \in C^\infty(\mathbb{R})$, and let $\epsilon_1, \ldots, \epsilon_N$ be non-zero constants, with $\sum \epsilon_n = 0$. We equip $\mathfrak{A}_N$ with the constant Poisson bracket:

$$\{F,G\}_{\mathfrak{A}_N} = -\sum_{n=1}^{N} \frac{1}{\epsilon_n} \int dx\, \frac{\delta F}{\delta a^{(n)}} \frac{\partial}{\partial x} \frac{\delta G}{\delta a^{(n)}}. \tag{4.5.8}$$

The *waterbag distribution function* corresponding to $a^{(1)}(x), \ldots, a^{(N)}(x)$ is defined as [195]:

$$f(x,p,t) = \sum_{n=1}^{N-1} C_n \mathbb{1}_{\left[a^{(n)}(x,t), a^{(n+1)}(x,t)\right]}(p), \tag{4.5.9}$$

where the C_n are constants and $\mathbb{1}_{[a,b]}$ is the characteristic function on the interval $[a,b]$ (see figure 4.2). We set $C_0 = C_N = 0$ by convention. Since f always evolves according to a Liouville equation on $T^*\mathbb{R}$, which is the same as an incompressible fluid motion in two dimensions, we expect that the time evolution of f (4.5.9) can be formulated entirely in terms of the boundaries $[a^{(n)}(x,t), a^{(n+1)}(x,t)]$ of the waterbags, so that the ansatz (4.5.9) holds at all times. Mathematically, we would like to say that the image of the map $a^{(1)}(x), \ldots, a^{(N)}(x) \mapsto f$ constitutes a Poisson submanifold of $C^\infty(T^*\mathbb{R})$. However, such f is not differentiable, so we do not quite have a map $\mathfrak{A}_N \to C^\infty(T^*\mathbb{R})$. This problem can be sidestepped if we consider instead a map $\mathcal{W} : \mathfrak{A}_N \to \mathfrak{S}^*(\mathbb{R})$ into the space of moments. The p-moments of the waterbag distribution function f (4.5.9) are

$$A^{(k)} = \int dp\, p^k f = \frac{1}{k+1} \sum_{n=1}^{N} \left(C_{n-1} - C_n\right) \left(a^{(n)}\right)^{k+1}. \tag{4.5.10}$$

Identifying $\epsilon_n = C_{n-1} - C_n$ leads us to the following construction:

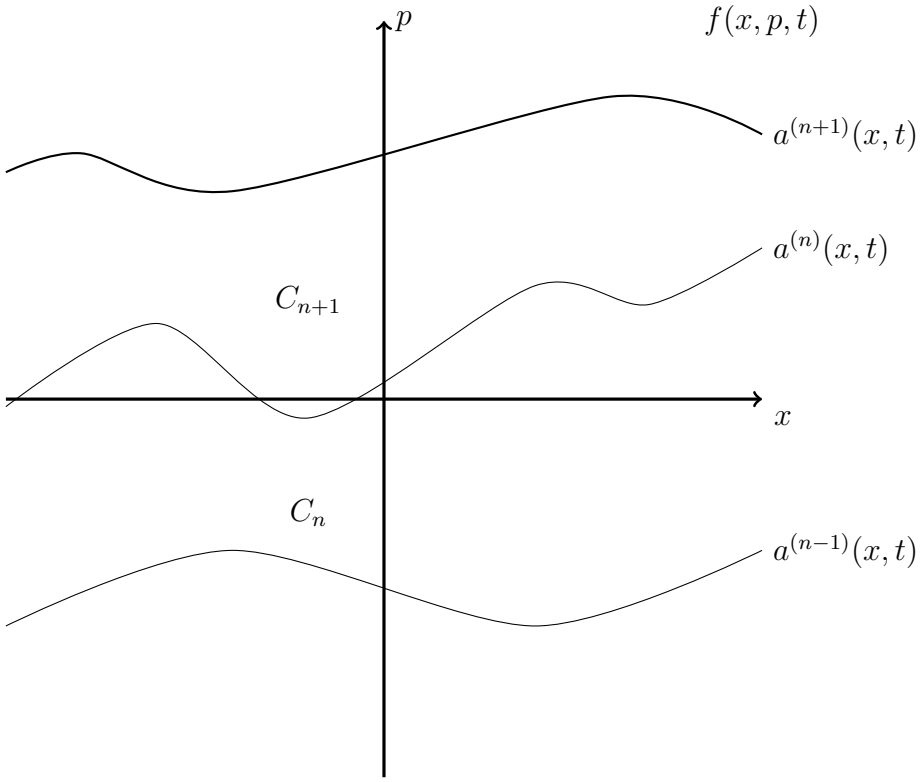


Figure 4.2: Example of a waterbag distribution f (4.5.9).

Proposition 4.6. *The* waterbag map $\mathcal{W} : \mathfrak{A}_N \to \mathfrak{S}^*(\mathbb{R})$*, defined by*

$$\mathcal{W} : \left(a^{(1)}, \dots, a^{(N)}\right) \mapsto \left(A^{(0)}, A^{(1)}, \dots\right), \quad A^{(k)} = \frac{1}{k+1} \sum_{n=1}^{N} \epsilon_n \left(a^{(n)}\right)^{k+1}. \tag{4.5.11}$$

is a Poisson map with respect to the bracket (4.5.8) on $\mathfrak{A}_N$ *and the one-dimensional Kuperschmidt–Manin bracket (4.5.7) on* $\mathfrak{S}^*(\mathbb{R})$*.*

Proof. Let $F = \tilde{F} \circ \mathcal{W}$ and $G = \tilde{G} \circ \mathcal{W}$. By the functional chain rule we have

$$\frac{\delta F}{\delta a^{(n)}} = \sum_{k=0}^{\infty} \frac{\delta \tilde{F}}{\delta A^{(k)}} \epsilon_n \left(a^{(n)}\right)^k, \tag{4.5.12}$$

so

$$\begin{aligned}
\{F,G\}_{\mathfrak{A}_N} &= -\int dx\ \sum_{n=1}^{N}\frac{1}{\epsilon_n}\sum_{k,l=0}^{\infty}\frac{\delta\tilde{F}}{\delta A^{(k)}}\epsilon_n\left(a^{(n)}\right)^k\frac{\partial}{\partial x}\left(\frac{\delta G}{\delta A^{(l)}}\epsilon_n\left(a^{(n)}\right)^l\right),\\
&= -\int dx\ \sum_{k,1=0}^{\infty}\sum_{n=1}^{N}\Big(\epsilon_n\left(a^{(n)}\right)^{k+1}\frac{\delta\tilde{F}}{\delta A^{(k)}}\frac{\partial}{\partial x}\frac{\delta\tilde{G}}{\delta A^{(l)}}\\
&\qquad\qquad + \epsilon_n l\left(a^{(n)}\right)^{k+l-1}\frac{\partial a^{(n)}}{\partial x}\frac{\delta\tilde{F}}{\delta A^{(k)}}\frac{\delta\tilde{G}}{\delta A^{(l)}}\Big),\\
&= -\int dx\ \sum_{k,l=0}^{\infty}\frac{\delta\tilde{F}}{\delta A^{(k)}}\left((k+l)A^{(k+l-1)}\frac{\partial}{\partial x}\frac{\delta\tilde{G}}{\delta A^{(l)}} + l\frac{\delta\tilde{G}}{\delta A^{(l)}}\frac{\partial A^{(k+l-1)}}{\partial x}\right)\\
&= \{\tilde{F},\tilde{G}\}_{KM}\circ\mathcal{W}, \qquad (4.5.13)
\end{aligned}$$

where we have used the definition of $\mathcal{W}$ (4.5.11) in the second-to-last line. Thus $\mathcal{W}$ is a Poisson map. □

The original application of the waterbag map comes from the reduction of the *Benney hydrodynamic chain* or *Benney moment equations* [15]

$$\frac{\partial A^{(n)}}{\partial t} + \frac{\partial A^{(n+1)}}{\partial x} + nA^{(n-1)}\frac{\partial A^{(0)}}{\partial x} = 0. \qquad (4.5.14)$$

The Benney moment equations are the moment equations for a Vlasov-like system

$$\frac{\partial f}{\partial t} + p\frac{\partial f}{\partial x} - \frac{\partial}{\partial x}\left(\int_{-\infty}^{\infty}dp\ f\right)\frac{\partial f}{\partial p} = 0. \qquad (4.5.15)$$

Equations (4.5.14) and (4.5.15) are Hamiltonian systems, with the respective Hamiltonian functionals being

$$H_{Benney}\left[A^{(0)},A^{(1)},\ldots\right] = \frac{1}{2}\int dx\ \left(A^{(2)} + \left(A^{(0)}\right)^2\right), \qquad (4.5.16)$$

$$H_f[f] = \frac{1}{2}\int dxdp\ \left(p^2 + \left(\int dp' f(x,p')\right)\right)f(x,p), \qquad (4.5.17)$$

with $\iota_{mom}^* H_{Benney} = H_f$. The corresponding equations in the waterbag variables are

$$\frac{\partial a^{(n)}}{\partial t} + a^{(n)}\frac{\partial a^{(n)}}{\partial x} + \sum_{m=1}^{N}\epsilon_m\frac{\partial a^{(m)}}{\partial x} = 0, \qquad (4.5.18)$$

which is a Hamiltonian system with the Hamiltonian functional

$$\begin{aligned}
H_a\left[a^{(1)},\ldots,a^{(N)}\right] &= \mathcal{W}^* H_{Benney}\\
&= \int dx\ \left(\frac{1}{6}\sum_{n=1}^{N}\epsilon_n\left(a^{(n)}\right)^3 + \frac{1}{2}\sum_{n,m=1}^{N}\epsilon_n\epsilon_m a^{(n)}a^{(m)}\right), \qquad (4.5.19)
\end{aligned}$$

with the Poisson bracket (4.5.8) on $\mathfrak{A}_N$. The waterbag map $\mathcal{W}$ (4.5.11) can also be used to reduce the one-dimensional Vlasov–Poisson system, although we need to change one of the waterbag variables to the electric potential φ (4.2.15) [144].

4.6 Conclusion and future directions

This chapter aims to investigate the relationship between the Hamiltonian structures at different levels of description for a possibly charged dilute monatomic gas. In section **4.1** we reviewed the hierarchy of kinetic descriptions of the gas and the Hamiltonian reductions along the hierarchy. In section **4.2** we studied the hydrodynamic variables known as raw moments or Vlasov moments. The space of moments is a Poisson manifold equipped with the Kuperschmidt–Manin bracket, and the map from distribution functions to moments is a Poisson map. We encounter our first instance of the *moment closure problem* in gas kinetic theory, where one cannot arrive at a closed and finite system of hydrodynamic variables without approximation. We then introduced another class of Poisson maps involving generalised entropy variables in section **4.3**, and discussed their application in approximate Hamiltonian reduction in section **4.4**. We find that ignoring the contribution from the relative entropy density $r[f|f_m]$ (4.4.8) of f against its local Maxwellian f_m (4.4.5) in the kinetic-theory Hamiltonian (4.4.2) leads to an approximate reduction of the collisionless Boltzmann equation to the compressible Euler equations (Proposition 4.3), and similarly for the Vlasov–Poisson equation (Corollary 4.1). Finally, we also discussed hydrodynamic reductions from singular Poisson submanifolds in the space of kinetic distribution functions in section **4.5**.

The interest in hydrodynamic reductions of kinetic theory is mainly driven by applications in plasma theory, where hydrodynamic models are much sought after. Recently, there has also been an interest in applying kinetic theory to the galactic dynamics, where the Jeans equation for a self-gravitating stellar system interacting under a mean field is considered [19, 36, 37, 93]. In these applications the *action-angle variables* $(\theta^1 \ldots, \theta^n, J_1, \ldots, J_n)$ for the $2n$-dimensional phase space S are used [10, 118]. The action variables J_i are in involution $\{J_i, J_j\} = 0$, and compact level sets $J_i = a_i$ where $dJ_1, \ldots, dJ_n$ are linearly independent are diffeomorphic to an n-torus $\mathbb{T}^n$. We can describe the level sets with periodic coordinates $(\theta^1 \ldots, \theta^n)$, and the symplectic form on S near each level set is $\omega = d\theta^i \wedge dJ_i$. Kinetic theory on the action-angle phase space S is often formulated in terms of a distribution function $f = f_0(\mathbf{J}, \epsilon^2 t) + \epsilon f_1(\boldsymbol{\theta}, \mathbf{J}, t)$, where ϵ is a small parameter. This decomposition is known as "quasilinear theory", which originated from plasma theory [54, 181]. The Jeans

equation is often written in the following form

$$\frac{\partial f}{\partial t} = \{H_0(\mathbf{J}) + H_1[\epsilon f_1](\boldsymbol{\theta}, \mathbf{J}, t), f\}\,, \tag{4.6.1}$$

with the aim of studying the slow evolution of $f_0(\mathbf{J}, \epsilon^2 t)$ through averaging over the fast f_1-evolution and also the fast angle variables. Mathematically, we should think of the action variables $\mathbf{J}$ as the moment map $m_T : S \to \mathbb{R}^n$ of a Hamiltonian $\mathbb{T}^n$-action. A compact connected symplectic manifolds S admitting an effective[7] Hamiltonian $\mathbb{T}^n$-action is called a *symplectic toric manifold*, and is a well-studied object in symplectic geometry [27, 83]. The image $\Delta = m_T(S) \subset \mathbb{R}^n$ is a convex polytope known as the *moment polytope* (Atiyah–Guillemin–Sternberg) [12, 85], and conversely the symplectic manifold S can be recovered from the moment polytope Δ (Delzant) [47]. The moment map $m_T : S \to S/\mathbb{T}^n = \Delta$ is a fibration, and the fibre at a point $\mathbf{J} \in \Delta$ on a k-dimensional face is a k-dimensional torus. In particular, S admits a degenerate system of action-angle coordinates $(\theta^1 \ldots, \theta^n, J_1, \ldots, J_n)$ that are only non-degenerate on $m_T^{-1}(\mathrm{Int}\Delta)$, so symplectic toric manifolds can be considered as generalised spaces where the kinetic theory of self-gravitating stellar systems can be formulated on. We can consider reductions from $f \in C^\infty(S)$ to $f_0 \in C^\infty(\Delta)$ instead of the hydrodynamic reductions from cotangent bundle distribution functions $f \in C^\infty(T^*M)$ to sections of vector bundles $(m, \rho, \ldots) \in \Gamma(E)$ over M studied in this chapter. Note however that the techniques used in this chapter do not carry over without significant modification, as the space $\mathbb{R}^n$ of action variables $\mathbf{J}$ is the dual space of an abelian Lie algebra, so the Poisson structure it carries is trivial. The slow evolution in $f_0(\mathbf{J}, \epsilon^2 t)$ has also been described as diffusive in the literature [36], so a double bracket formulation (see section **2.4.5**) is needed – it would be interesting to study these diffusion terms in terms of the moment map m_T.

A separate line investigation would be to look at quantum mechanics. There are several formulations of non-relativistic quantum mechanics that share similarities with fluid dynamics and kinetic theory. One such related formulation is the *phase-space formulation* of quantum mechanics [81, 139, 184, 188] (see also [29, 88, 196] for modern reviews). For a system on $\mathbb{R}^n$, one uses a complex phase space function $f(x, p, t)$ instead of the pure density operator $|\Psi\rangle\langle\Psi|$ and uses the associative but non-commutative *Moyal star product*

$$f * g = f \exp\left(\frac{\mathrm{i}\hbar}{2}\left(\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}\right)\right) g \tag{4.6.2}$$

in place of operator multiplication, where the direction of the arrow indicates the argument that the partial derivative acts on. Under suitable regularity assumptions, the space of complex phase-space functions equipped with the Moyal star product is isomorphic to the

[7] By effective we mean that the group homomorphism $\mathbb{T}^n \to \mathrm{Diff}(S)$ induced by the $\mathbb{T}^n$-action is injective.

space of operators on $\mathbb{R}^n$ as associative algebras, and the isomorphism is known as the *Wigner–Weyl transform*. In particular, the trace of operators correspond to the phase space integral $\int dV$ of functions under a suitable normalisation. The operator commutator is replaced by the *Moyal bracket*

$$\{\{f,g\}\} = \frac{f*g-g*h}{\mathrm{i}\hbar} = \frac{\partial f}{\partial x}\frac{\partial g}{\partial p} - \frac{\partial f}{\partial p}\frac{\partial g}{\partial x} + O(\hbar^2), \tag{4.6.3}$$

which agrees with the canonical Poisson bracket on $\mathbb{R}^{2n}$ to leading order in $\hbar$. The construction of Moyal star products from Poisson algebras is known as *deformation quantisation*, and has been achieved on general symplectic manifolds (Fedosov) [62] and on general Poisson manifolds (Kontsevich) [110]. Our interest in the phase-space formulation of quantum mechanics is on whether the maps $\mathcal{G}_A^{pol}$ (4.3.36) can be adapted to this setting, perhaps through replacing ordinary products with Moyal products (4.6.2). Taking the p-integral $\int d^n p$ of a phase-space function can be considered as a partial trace, and it would be interesting to see whether some approximate hydrodynamic description using commuting x-dependent fields only exists.

Another related formulation is *quantum hydrodynamics*. The Madelung transform $\Psi(x,t) = D(x,t)\exp(\mathrm{i}\phi(x,t)/\hbar)$ leads to a description of quantum mechanics similar to the compressible Euler equations in potential flow (see sections **2.6.1.2** and **2.6.1.5**) [66, 106, 190]. Quantum mechanics can be formulated as a classical, infinite-dimensional Hamiltonian system using the canonical symplectic form on complex Hilbert spaces [38], and the map $\Psi \mapsto (m = D\nabla\phi, \rho = D)$ has been shown to be a Poisson map. We are interested in whether there is a "kinetic theory" for these quantum hydrodynamic formulations, a setting that allows us to extend the techniques in this chapter. Of course, both the phase-space formulation and the quantum hydrodynamic formulation of quantum mechanics have a common origin, namely the standard Hilbert space formulation of quantum mechanics, but it would be interesting to see whether these formulations are connected in other ways.

Chapter 5

Magnetohydrodynamic formulation for active rod suspensions

This chapter studies the analogy between MHD and the dynamics of a suspension of active rod-like swimmers. The material in this chapter is based on an unpublished manuscript written by the author.

5.1 Introduction

The dynamics of *active suspensions* has been a topic of much recent interest in soft matter physics [52, 53, 75, 90, 147, 162, 175]. An active suspension is a suspension of axis-symmetric swimming bacteria in a Newtonian fluid. In certain ideal limits where elastic liquid crystal effects can be ignored, the orientations of the swimmers evolve according to *Jeffery's equation* [82, 99, 101, 146]. These swimmers in turn exert an *active stress* on the fluid, leading to a closed system of evolution equations typical to a complex fluid.

This chapter studies the theoretical similarities between an active suspension of *rod-like* swimmers and magnetohydrodynamics [22, 113, 169]. We show that the governing equations for an active rod suspension are identical to that of MHD in an electromagnetically nonlinear medium [113, 158] (section **5.2.2**). In the inviscid limit, the active rod system admits a noncanonical Hamiltonian formulation that uses the same Poisson bracket as ordinary MHD, but has a different Hamiltonian functional (section **5.3.1**). The active rod system also admits a *Clebsch potential formulation*, just like ordinary MHD [133, 169] (section **5.3.2**), but possesses a larger class of gauge transformations (section **5.3.3**).

The properties of the solutions to the active rod system shares many similarities with MHD. A suspension of contractile active rods possess both linear and nonlinear *Alfvén wave* solutions (section **5.4**), a property ubiquitous to MHD and its various extensions [2, 3, 22, 169, 194]. We also obtain variational principles for these Alfvén wave solutions

using the *energy-Casimir* and *energy-momentum methods* (cf. section **2.4.2**). Finally, we study the static force-free equilibrium of the active rod system. These equilibria correspond to *force-free fields* in MHD, and we obtain variational principles analogous to those in MHD for these equilibria [151, 173, 191] (section **5.5**).

In this chapter, we focus on fluids on domains $M = \mathbb{R}^3$ or $\mathbb{R}^2$ and revert to vector calculus notation.

5.2 Governing equations

In this section we describe the governing equations for a dilute suspension of active rod-like swimmers. The time evolution of the orientations of the swimmers is described by *Jeffery's equation* [82, 99, 101, 146], and these swimmers exert a stress known as the *active stress* on the fluid [52, 53, 75, 90, 147, 162, 175]. We establish an analogy between these governing equations and the MHD equations in an electromagnetically nonlinear medium [113, 158].

5.2.1 Jeffery's equation and active stress

The time evolution of a suspension of axis-symmetric rigid bodies in an incompressible fluid is described by Jeffery's equation [99, 101, 146]. Let $\mathbf{n}$ be a unit vector field describing the orientation of the suspended bodies. Given a fluid velocity field $\mathbf{u}$, the director field $\mathbf{n}$ evolves as

$$\partial_t \mathbf{n} + \mathbf{u} \cdot \nabla \mathbf{n} = \mathbf{\Omega} \cdot \mathbf{n} + \beta \left(\mathbf{I} - \mathbf{nn} \right) \cdot \mathbf{E} \cdot \mathbf{n}, \tag{5.2.1}$$

where $\mathbf{I}$ is the identity tensor, β is the Bretherton parameter [25], $\mathbf{\Omega} = (-\nabla \mathbf{u} + (\nabla \mathbf{u})^T)/2$ is the vorticity field, and $\mathbf{E} = (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)/2$ is the strain field. Our convention is that the components of $\nabla \mathbf{u}$ are $\nabla_i u_j$. For rigid ellipsoids, $\beta = (1 - r^2)/(1 + r^2)$, where r is the aspect ratio, so $\beta = 1$ corresponds to rods and $\beta = -1$ corresponds to discs.

Jeffery's equation (5.2.1) can also be formulated in terms of the unnormalised director field $\mathbf{B} = |\mathbf{B}|\mathbf{n}$ ([82] p.75, [146] p.11–12). The time evolution of $\mathbf{B}$ is

$$\partial_t \mathbf{B} + \mathbf{u} \cdot \nabla \mathbf{B} = \mathbf{\Omega} \cdot \mathbf{B} + \beta \mathbf{E} \cdot \mathbf{B}, \tag{5.2.2}$$

which is equivalent to (5.2.1) except that we have introduced a magnitude degree of freedom $|\mathbf{B}|$, which evolves as

$$\partial_t \log|\mathbf{B}| + \mathbf{u} \cdot \nabla \log|\mathbf{B}| = \beta \mathbf{E} : \frac{\mathbf{BB}}{|\mathbf{B}|^2}. \tag{5.2.3}$$

Now consider the time evolution of the fluid velocity field $\mathbf{u}$. The suspended bodies exert a stress $\boldsymbol{\sigma}^{(n)}$ on the fluid. The momentum equation of the fluid is

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \nu \nabla^2 \mathbf{u} + \nabla \cdot \boldsymbol{\sigma}^{(n)}, \qquad \nabla \cdot \mathbf{u} = 0, \tag{5.2.4}$$

where P is the pressure and ν is the viscosity of the fluid. Equation (5.2.4) is simply the Navier–Stokes equation with an additional stress term $\boldsymbol{\sigma}^{(n)}$. The system (5.2.2, 5.2.4) is a typical internal state variable model for a complex fluid (cf. section **3.1**), where the internal state is completely characterised by the unit director field $\mathbf{n}$.

In [52, 53, 75, 90, 147, 162, 175], the following form for the suspension-induced stress is suggested as a model for an active suspension of axis-symmetric swimmers:

$$\boldsymbol{\sigma}^{(n)} = \kappa \mathbf{n}\mathbf{n}, \tag{5.2.5}$$

where κ is the *active parameter*. Systems with $\kappa < 0$ are called extensile, corresponding to a suspension of pushers, and systems with $\kappa > 0$ are called contractile, corresponding to a suspension of pullers.

In the following we will focus on suspensions of rod-like ($\beta = 1$) active swimmers in the inviscid ($\nu \to 0$) limit. The governing equations for such a suspension are

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \kappa \nabla \cdot \frac{\mathbf{B}\mathbf{B}}{|\mathbf{B}|^2}, \qquad \nabla \cdot \mathbf{u} = 0, \tag{5.2.6a}$$

$$\partial_t \mathbf{B} + \mathbf{u} \cdot \nabla \mathbf{B} = \mathbf{B} \cdot \nabla \mathbf{u}. \tag{5.2.6b}$$

The system (5.2.6a,b) is the object of study for the rest of the section. As we shall see, the system (5.2.6a,b) resembles the incompressible MHD equations in an electromagnetically nonlinear medium.

5.2.2 Analogy with MHD in a nonlinear medium

Consider an incompressible, conducting fluid that is polarisable and magnetisable. The electrodynamics of this fluid is described by Maxwell's equations in matter [96, 113]:

$$\nabla \cdot \mathbf{D} = \rho_f, \tag{5.2.7a}$$

$$\nabla \cdot \mathbf{B} = 0, \tag{5.2.7b}$$

$$\nabla \times \mathbf{H} = \mathbf{J}_f + \partial_t \mathbf{D}, \tag{5.2.7c}$$

$$\nabla \times \mathbf{E} + \partial_t \mathbf{B} = 0, \tag{5.2.7d}$$

where $\mathbf{E}$ is the electric field, $\mathbf{B}$ is the magnetic field, $\mathbf{D}$ is the displacement field, $\mathbf{H}$ is the induction field, ρ_f is the free charge density, and $\mathbf{J}_f$ is the free current density. On the other hand, the momentum equation of such a fluid is

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \nu \nabla^2 \mathbf{u} + \mathbf{f}_L, \qquad \nabla \cdot \mathbf{u} = 0, \tag{5.2.8}$$

where $\mathbf{f}_L$ is the Lorentz force per unit volume:

$$\mathbf{f}_L = \rho_f \mathbf{E} + \mathbf{J}_f \times \mathbf{B}. \tag{5.2.9}$$

As in ordinary MHD (see e.g. [22, 113]), we assume that the system is quasineutral, and that the free current obeys Ohm's law:

$$\rho_f = 0, \qquad \mathbf{J}_f = \frac{1}{\eta} \left(\mathbf{E} + \mathbf{u} \times \mathbf{B} \right), \tag{5.2.10}$$

where η is the resistivity. In the non-relativistic limit, we can ignore the displacement current term $\partial_t \mathbf{D}$ in the Maxwell-Ampère equation (5.2.7c). The Lorentz force $\mathbf{f}_L$ (5.2.9) is then

$$\mathbf{f}_L = (\nabla \times \mathbf{H}) \times \mathbf{B} = -(\nabla \mathbf{H}) \cdot \mathbf{B} + \mathbf{B} \cdot \nabla \mathbf{H}. \tag{5.2.11}$$

The non-relativistic Maxwell-Ampère equation can also be used to solve for $\mathbf{E}$:

$$\mathbf{E} = -\mathbf{u} \times \mathbf{B} + \eta \nabla \times \mathbf{H}, \tag{5.2.12}$$

which gives an evolution equation for $\mathbf{B}$ using Faraday's law (5.2.7d)

$$\partial_t \mathbf{B} = \nabla \times (\mathbf{u} \times \mathbf{B}) - \eta \nabla \times \nabla \times \mathbf{H}, \qquad \nabla \cdot \mathbf{B} = 0. \tag{5.2.13}$$

The system (5.2.8, 5.2.13) describes the time evolution of a MHD system in an electromagnetically nonlinear medium [113, 158]. It is closed subject to a constitutive relation of the form $\mathbf{H} = \mathbf{H}(\mathbf{B}, \nabla \mathbf{B}, \ldots)$. The vacuum relation $\mathbf{H} = \mathbf{B}$ returns ordinary MHD.

Let us specialise to constitutive relations of the form $\mathbf{H} = \partial h(|\mathbf{B}|^2)/\partial \mathbf{B}$, in which case we can write $\mathbf{f}_L$ as the divergence of a Maxwell stress (using $\nabla \cdot \mathbf{B} = 0$):

$$\mathbf{f}_L = \nabla \cdot \boldsymbol{\sigma}_L, \qquad \boldsymbol{\sigma}_L = -g(|\mathbf{B}|^2)\mathbf{I} + 2h'(|\mathbf{B}|^2)\mathbf{B}\mathbf{B}, \tag{5.2.14}$$

where $g(x) = h(x) + \int^x 2y h''(y) dy$. Remarkably, the choice

$$h(|\mathbf{B}|^2) = \frac{\kappa}{2} \log(|\mathbf{B}|^2) \tag{5.2.15}$$

gives a momentum equation (5.2.8) identical to that of a fluid suspension (5.2.4) with the active stress (5.2.5). The Maxwell stress $\boldsymbol{\sigma}_L$ (5.2.14) only differs from the active stress (5.2.5) by a term proportional to $\mathbf{I}$, which can be absorbed into the pressure P.

The evolution equation (5.2.13) for $\mathbf{B}$ is also remarkably similar to Jeffery's equation for rods (5.2.6b) in the non-resistive ($\eta \to 0$) limit. We can rewrite (5.2.13) as (using $\nabla \cdot \mathbf{u} = \nabla \cdot \mathbf{B} = 0$)

$$\partial_t \mathbf{B} + \mathbf{u} \cdot \nabla \mathbf{B} = \mathbf{B} \cdot \nabla \mathbf{u}, \qquad \nabla \cdot \mathbf{B} = 0, \tag{5.2.16}$$

which is identical to (5.2.6b), expect that $\nabla \cdot \mathbf{B} = 0$ is required. Note that if $\mathbf{B}(t = 0)$ is divergence-free, it will remain divergence-free under the evolution equation (5.2.6b) for any choice of (divergence-free) $\mathbf{u}$. Thus there is an exact analogy between the active rod system (5.2.6a,b) and a MHD system a nonlinear medium, provided the unnormalised director field $\mathbf{B} = |\mathbf{B}|\mathbf{n}$ is chosen to be divergence-free at $t = 0$.

5.3 Hamiltonian formulation of the active rod system

In this section we show that the active rod system (5.2.6a,b) is in fact a noncanonical Hamiltonian system, with the same Hamiltonian structure as the incompressible MHD equations but a different expression for the magnetic energy. The main difference between the active rod system (5.2.6a,b) and the nonlinear MHD system (5.2.8, 5.2.13) is that, while the unnormalised director $\mathbf{B}$ for the active rods has a spurious magnitude degree of freedom $|\mathbf{B}|$, the magnetic field $\mathbf{B}$ in the nonlinear MHD system is required to be divergence-free, which removes a different degree of freedom. We can accommodate both conditions with the *Clebsch potential formulation* [133, 155, 169, 193] where $\mathbf{B}$ is manifestly divergence-free, and obtain *gauge transformations* of the Clebsch potentials that correspond to rescaling $|\mathbf{B}|$.

5.3.1 Noncanonical Hamiltonian formulation

The active rod system (5.2.6a,b) can be formulated as a noncanonical Hamiltonian system on the space $\mathfrak{m}_\mu^*$ of incompressible MHD variables $(\mathbf{u}, \mathbf{B})$ (see section **2.6.2.2**). The explicit expression for the Poisson bracket is (2.6.38)

$$\begin{aligned}\{F, G\} = -\int d^3x\, \mathbf{u} \cdot \left(\frac{\delta F}{\delta \mathbf{u}} \cdot \nabla \frac{\delta G}{\delta \mathbf{u}} - \frac{\delta G}{\delta \mathbf{u}} \cdot \nabla \frac{\delta F}{\delta \mathbf{u}} \right) \\ + \mathbf{B} \cdot \left(\frac{\delta F}{\delta \mathbf{u}} \cdot \nabla \frac{\delta G}{\delta \mathbf{B}} + \left(\nabla \frac{\delta F}{\delta \mathbf{u}} \right) \cdot \frac{\delta G}{\delta \mathbf{B}} - \frac{\delta G}{\delta \mathbf{u}} \cdot \nabla \frac{\delta F}{\delta \mathbf{B}} - \left(\nabla \frac{\delta G}{\delta \mathbf{u}} \right) \cdot \frac{\delta F}{\delta \mathbf{B}} \right).\end{aligned} \tag{5.3.1}$$

Given a Hamiltonian functional H, the evolution equations are

$$\partial_t \mathbf{u} = -\nabla P - \left(\nabla \frac{\delta H}{\delta \mathbf{u}} \right) \cdot \mathbf{u} - \nabla \cdot \left(\frac{\delta H}{\delta \mathbf{u}} \mathbf{u} \right) - \left(\nabla \frac{\delta H}{\delta \mathbf{B}} \right) \cdot \mathbf{B} + \nabla \cdot \left(\mathbf{B} \frac{\delta H}{\delta \mathbf{B}} \right), \tag{5.3.2a}$$

$$\partial_t \mathbf{B} = -\nabla \cdot \left(\frac{\delta H}{\delta \mathbf{u}} \mathbf{B} \right) + \mathbf{B} \cdot \nabla \frac{\delta H}{\delta \mathbf{u}}, \tag{5.3.2b}$$

where P is an arbitrary function that enforces the constraint $\nabla \cdot \mathbf{u} = 0$. The Poisson bracket (5.3.1) makes sense regardless of whether the divergence-free condition $\nabla \cdot \mathbf{B} = 0$ hold, but $\nabla \cdot \mathbf{B} = 0$ is preserved by (5.3.2b) for *any* Hamiltonian if it holds at $t = 0$. The active rod system (5.2.6a,b) can be written in the form (5.3.2a,b) above with the following choice for the Hamiltonian:

$$H_a\left[\mathbf{u}, \mathbf{B}\right] = \int d^3x \, \frac{1}{2}|\mathbf{u}|^2 + \frac{\kappa}{2}\log|\mathbf{B}|^2. \tag{5.3.3}$$

We can think of the term $h(|\mathbf{B}|^2) = (\kappa/2)\log(|\mathbf{B}|^2)$ as the "magnetic energy density" of the active rod suspension, using our analogy between active rod suspensions and MHD in a nonlinear medium.

One then wonders why the physically spurious magnitude degree of freedom $|\mathbf{B}|$ appears in the Hamiltonian (5.3.3) for the active rod system (5.2.6a,b), even if the active rod system can be written in terms of the normalised director field $\mathbf{n} = \mathbf{B}/|\mathbf{B}|$ only. We establish $|\mathbf{B}|$ as a *gauge degree of freedom* that can be removed in the actual evolution equations, but needs to be kept in the Hamiltonian formulation. Consider a time-independent rescaling

$$\mathbf{B}(\mathbf{x}, t) \mapsto \mathbf{B}'(\mathbf{x}, t) = \mathrm{e}^{\mathcal{B}(\mathbf{x})}\mathbf{B}(\mathbf{x}, t), \tag{5.3.4}$$

which we call a *gauge transformation* $g_{\mathcal{B}} : \mathfrak{m}_\mu^* \to \mathfrak{m}_\mu^*$, and denote the group of gauge transformations (5.3.4) by $\mathcal{G}$. These gauge transformations are not quite Poisson automorphisms, as we can show by direct computation that

$$\begin{aligned}\{g_{\mathcal{B}}^* F, g_{\mathcal{B}}^* G\} =& g_{\mathcal{B}}^*\{F, G\} - \int d^3x \, \left(\mathbf{B} \cdot \frac{\delta G}{\delta \mathbf{B}}\frac{\delta F}{\delta \mathbf{u}} - \mathbf{B} \cdot \frac{\delta F}{\delta \mathbf{B}}\frac{\delta G}{\delta \mathbf{u}}\right) \cdot \nabla \mathcal{B} \\ =& g_{\mathcal{B}}^*\{F, G\} - T_{\mathcal{B}}[F, G].\end{aligned} \tag{5.3.5}$$

If F depends on $\mathbf{B}$ through $\mathbf{n}$ only, or equivalently that $g_{\mathcal{B}}^* F = F$ for all $g_{\mathcal{B}} \in \mathcal{G}$, then

$$\frac{\delta F[\mathbf{u}, \mathbf{n}]}{\delta \mathbf{B}} = \frac{1}{|\mathbf{B}|}\left(\mathbf{I} - \mathbf{n}\mathbf{n}\right) \cdot \frac{\delta F}{\delta \mathbf{n}}, \tag{5.3.6}$$

and in particular $\mathbf{B} \cdot \delta F/\delta \mathbf{B} = 0$. So we have $T_{\mathcal{B}}[F, G] = 0$ for $F = F[\mathbf{u}, \mathbf{n}], G = G[\mathbf{u}, \mathbf{n}]$, and thus the space of $\mathcal{G}$-fixed functionals $\mathcal{F}(\mathfrak{m}_\mu^*)^{\mathcal{G}}$ form a Poisson subalgebra. This induces a Poisson bracket on $\mathfrak{m}_\mu^*/\mathcal{G}$, the space for the variables $(\mathbf{u}, \mathbf{n})$ (cf. (2.5.6, 2.5.7), section **2.5.1**). This construction is applied in [16, 17, 57] to find Poisson brackets for normalised director fields and normalised $\mathbf{Q}$-tensors[1].

[1]The $\mathbf{Q}$-tensor formulation will be discussed in greater detail in section **5.6**.

The active Hamiltonian (5.3.3) transforms by the addition of a time-independent constant $H_a \mapsto H_a + C$, which in particular is a Casimir functional:

$$g_{\mathcal{B}}^* H_a = H_a \left[\mathbf{u}, \mathrm{e}^{\mathcal{B}}\mathbf{B}\right] = H_a \left[\mathbf{u}, \mathbf{B}\right] + \kappa \int d^3x\, \mathcal{B}(\mathbf{x}), \tag{5.3.7}$$

which leaves the Hamiltonian flow X_{H_a} unchanged under this rescaling. We would like to show that $X_{H_a} = \{\cdot, H_a\}$ maps gauge-invariant functionals to gauge-invariant functionals, so that the noncanonical Hamiltonian system generated H_a induces a reduced system on the quotient $\mathfrak{m}_\mu^* \to \mathfrak{m}_\mu^*/\mathcal{G}$. If $\mathcal{G}$ were a group of Poisson automorphisms, the condition $g_{\mathcal{B}}^* H_a = H_a + C$ (C Casimir) for all $g_{\mathcal{B}} \in \mathcal{G}$ would be sufficient (cf. (5.3.23)). Fortunately, we have $\mathbf{B}\cdot\delta H_a/\delta\mathbf{B} = \kappa$, which is constant, so integrating by parts and using $\nabla\cdot(\delta F/\delta\mathbf{u}) = 0$ shows that $T_{\mathcal{B}}[F, H_a] = 0$ for any gauge-invariant $F \in \mathcal{F}(\mathfrak{m}_\mu^*)^{\mathcal{G}}$. Putting everything together, we have

$$g_{\mathcal{B}}^*\{F, H_a\} = \{g_{\mathcal{B}}^* F, g_{\mathcal{B}}^* H_a\} + T_{\mathcal{B}}[F, H_a] = \{F, H_a + C\} + 0 = \{F, H_a\}, \tag{5.3.8}$$

which shows that $X_{H_a} = \{\cdot, H_a\} : \mathcal{F}(\mathfrak{m}_\mu^*/\mathcal{G}) \to \mathcal{F}(\mathfrak{m}_\mu^*/\mathcal{G})$ is well-defined, thus proving gauge invariance. Note however that we could not have obtained the vector field X_{H_a} from any Hamiltonian system on the quotient Poisson manifold $\mathfrak{m}_\mu^*/\mathcal{G}$, because $\delta H[\mathbf{u}, \mathbf{n}]/\delta\mathbf{B}$ is always perpendicular to $\mathbf{n}$ (5.3.6) and thus can never give to a tensor structure of the form $\mathbf{nn}$ in the stress (cf. (5.3.2b)).

5.3.2 Clebsch potential formulation

In the unnormalised director formulation of the active rod equations (5.2.6a,b), we need to choose some arbitrary $\mathbf{B}$ parallel to the director field $\mathbf{n}$ initially. We can use *Clebsch potentials* to construct such $\mathbf{B}$ with $\nabla \cdot \mathbf{B} = 0$. Consider the following equation

$$\mathbf{n} \cdot \nabla\Psi = 0. \tag{5.3.9}$$

In three dimensions, we can find two independent local solutions Ψ_1, Ψ_2 to (5.3.9) as long as $\mathbf{n}$ does not vanish locally[2]. Since $\mathbf{n}$ is perpendicular to $\nabla\Psi_1, \nabla\Psi_2$, $\mathbf{n}$ is parallel to $\nabla\Psi_1 \times \nabla\Psi_2$. We can therefore take the unnormalised director field to be

$$\mathbf{B} = \nabla\Psi_1 \times \nabla\Psi_2, \tag{5.3.10}$$

which is divergence-free. In MHD, the functions Ψ_1, Ψ_2 are called the *Clebsch potentials* for the magnetic field $\mathbf{B}$ [133, 169]. Equation (5.3.10) is called a *Clebsch representation*

[2]This is a special case of the Frobenius theorem; see e.g. ch. 4 of [44]

of a divergence-free vector field $\mathbf{B}$. Each field line of $\mathbf{n}$ or $\mathbf{B}$ lies on the intersection of the surfaces $\Psi_1 = a, \Psi_2 = b$ for some real a, b, so it is common to think of the Clebsch potentials as labels for the field lines. Clebsch potentials are also sometimes called *flux labels* or *flux functions*, and the level surfaces $\Psi_i = a$ are called *flux surfaces*, since the flux of $\mathbf{B}$ through any patch of a level surface of Ψ_i is always zero [92].

Remark 5.1. It is not always possible to extend a locally-defined Clebsch representation to a global one. Notably, the representation (5.3.10) of $\mathbf{B}$ by globally defined, single-valued Clebsch potentials Ψ_1, Ψ_2 is not possible if $\mathbf{B}$ has nonzero *helicity* [133, 155, 193].

In the following we shall assume that a Clebsch representation (5.3.10) exists globally. If we impose that Ψ_1, Ψ_2 evolve in time as advected scalars

$$\partial_t \Psi_i + \mathbf{u} \cdot \nabla \Psi_i = 0, \qquad i = 1, 2, \tag{5.3.11}$$

then the corresponding $\mathbf{B} = \nabla\Psi_1 \times \nabla\Psi_2$ would evolve according (5.2.6b), assuming $\nabla \cdot \mathbf{u} = 0$ [68, 169, 191].

Similarly, in two dimensions, the equation (5.3.10) has one independent local solution Ψ provided $\mathbf{n}$ does not vanish locally. In this case taking

$$\mathbf{B} = \nabla_\times \Psi = (\partial_y \Psi, -\partial_x \Psi), \tag{5.3.12}$$

gives a divergence-free $\mathbf{B}$ parallel to $\mathbf{n}$, since $\nabla\Psi$ is perpendicular to $\mathbf{n}$. Again, if we impose that the Clebsch potential evolves in time as an advected scalar,

$$\partial_t \Psi + \mathbf{u} \cdot \nabla \Psi = 0, \tag{5.3.13}$$

the corresponding $\mathbf{B} = \nabla_\times \Psi$ evolves according to (5.2.6b) in two dimensions.

Let us illustrate the use of Clebsch potentials in modelling nematic geometry with an example in two dimensions. We can abandon the director field $\mathbf{n}$ entirely and model the orientation of the active rods using the contour lines of the Clebsch potential Ψ. At points where $\nabla\Psi = 0$, the director field $\mathbf{n}$ is no longer defined, but we can still make sense of the orientation using the contours of Ψ, allowing singular orientation fields such as defects to be described. For example, let

$$\Psi(x, y) = \Theta(x)x^2 + y^2, \quad \Theta(x) = \frac{\int_0^x g(s)g(1-s)ds}{\int_0^1 g(s)g(1-s)ds}, \quad g(s) = \begin{cases} 0 & s \le 0 \\ \exp(-1/s) & s > 0 \end{cases}, \tag{5.3.14}$$

so that $\Theta(x)$ is a smoothed step function with $\Theta(x < 0) = 0$ and $\Theta(x > 1) = 1$. We plot the contour lines of Ψ in figure 5.1 – Ψ models the geometry of a charge-$1/2$ defect at the origin [34, 67]. Note how $\mathbf{B} = \nabla_\times \Psi$ vanishes on the entire negative x-axis even though the plot shows that the orientation of the rods is along the x-axis at those points.

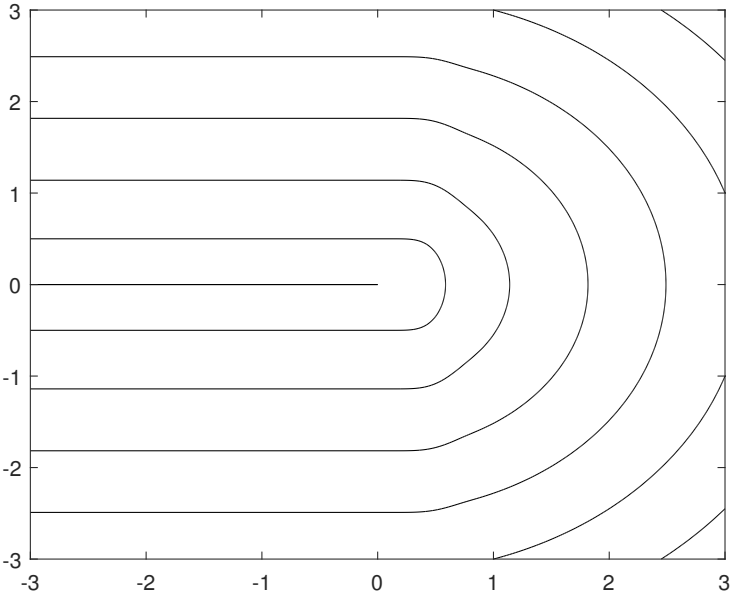


Figure 5.1: The contour lines of $\Psi(x, y) = \Theta(x)x^2 + y^2$ models the nematic geometry of a charge-$1/2$ defect.

5.3.3 Gauge transformations for Clebsch potentials

The Hamiltonian structure of the active rod system (5.2.6a,b) can also be expressed in terms of Clebsch potentials. The Clebsch potential formulation possesses a cleaner notion of gauge transformations, where the gauge group acts by Poisson automorphisms. Consider the following noncanonical Hamiltonian system for the variables $\mathbf{u}, \Psi_1, \Psi_2$, with Poisson bracket

$$\begin{aligned}\{F, G\} = -\int d^3x\, \mathbf{u} \cdot \left(\frac{\delta F}{\delta \mathbf{u}} \cdot \nabla \frac{\delta G}{\delta \mathbf{u}} - \frac{\delta G}{\delta \mathbf{u}} \cdot \nabla \frac{\delta F}{\delta \mathbf{u}} \right) \\ + \Psi_1 \left(\frac{\delta F}{\delta \mathbf{u}} \cdot \nabla \frac{\delta G}{\delta \Psi_1} - \frac{\delta G}{\delta \mathbf{u}} \cdot \nabla \frac{\delta F}{\delta \Psi_1} \right) \\ + \Psi_2 \left(\frac{\delta F}{\delta \mathbf{u}} \cdot \nabla \frac{\delta G}{\delta \Psi_2} - \frac{\delta G}{\delta \mathbf{u}} \cdot \nabla \frac{\delta F}{\delta \Psi_2} \right),\end{aligned} \tag{5.3.15}$$

and the active Hamiltonian

$$H_a[\mathbf{u}, \Psi_1, \Psi_2] = \int d^3x\, \frac{1}{2}|\mathbf{u}|^2 + \frac{\kappa}{2} \log|\nabla\Psi_1 \times \nabla\Psi_2|^2. \tag{5.3.16}$$

We recognise the Poisson bracket (5.3.15) as the $(-)$-Lie–Poisson bracket on the dual of the semidirect product Lie algebra $\mathrm{Vect}_\mu(\mathbb{R}^3) \ltimes C^\infty(\mathbb{R}^3, \mathbb{R}^2)$. The active Hamiltonian (5.3.16)

generates the following set of evolution equations ($i = 1, 2$):

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \kappa \nabla \cdot \frac{\mathbf{BB}}{|\mathbf{B}|^2}, \qquad \nabla \cdot \mathbf{u} = 0, \tag{5.3.17a}$$

$$\partial_t \Psi_i + \mathbf{u} \cdot \nabla \Psi_i = 0, \qquad \mathbf{B} = \nabla \Psi_1 \times \nabla \Psi_2, \tag{5.3.17b}$$

from which we recover (5.2.6a,b). There is a gauge degree of freedom associated to the Clebsch potentials that corresponds to the rescaling transformation of $\mathbf{B}$. Recall that each field line is labelled by $\Psi_1 = a, \Psi_2 = b$ for some real a, b. The geometry of the field lines is preserved under any smooth relabelling of the field lines. Such a smooth relabelling can be concretely represented by a diffeomorphism $(S_1, S_2) : \mathbb{R}^2 \to \mathbb{R}^2$:

$$S_1 = S_1(\Psi_1, \Psi_2), \qquad S_2 = S_2(\Psi_1, \Psi_2). \tag{5.3.18}$$

If we take S_1, S_2 as our new Clebsch potentials, we should recover the same geometrical configuration of the field lines. Indeed,

$$\nabla S_1 \times \nabla S_2 = \frac{\partial(S_1, S_2)}{\partial(\Psi_1, \Psi_2)} \nabla \Psi_1 \times \nabla \Psi_2, \tag{5.3.19}$$

and since the Jacobian determinant $\partial(S_1, S_2)/\partial(\Psi_1, \Psi_2)$ is nonzero everywhere for an invertible transformation, we see that the unnormalised director field defined by S_1, S_2 is parallel to that defined by Ψ_1, Ψ_2, resulting in the same geometry. In fact:

Proposition 5.1. *The gauge transformations (5.3.18) from the group* $\mathrm{Diff}(\mathbb{R}^2)$ *acts as Poisson automorphisms on the space* $(\mathrm{Vect}_\mu(\mathbb{R}^3) \ltimes C^\infty(\mathbb{R}^3, \mathbb{R}^2))^*$ *equipped with the Poisson bracket (5.3.15).*

Proof. We show that Poisson bracket (5.3.15) retains the same form under the change of variables $(\mathbf{u}, \Psi_1, \Psi_2) \mapsto (\mathbf{u}, S_1, S_2)$ induced by the gauge transformation (5.3.18). The first line of (5.3.15) retains the same form, so we only need to check this for the last two lines involving Ψ_1, Ψ_2. The terms on the last two lines of (5.3.15) proportional to $\delta F/\delta \mathbf{u}$

transform as

$$\begin{aligned}
&\int d^3x \ \begin{pmatrix}\Psi_1 & \Psi_2\end{pmatrix} \frac{\delta F}{\delta \mathbf{u}} \cdot \nabla \begin{pmatrix} \dfrac{\delta G}{\delta \Psi_1} \\ \dfrac{\delta G}{\delta \Psi_2} \end{pmatrix} \\
&= \int d^3x \ \begin{pmatrix}\Psi_1 & \Psi_2\end{pmatrix} \frac{\delta F}{\delta \mathbf{u}} \cdot \nabla \begin{pmatrix} \dfrac{\partial S_1}{\partial \Psi_1} & \dfrac{\partial S_2}{\partial \Psi_1} \\ \dfrac{\partial S_1}{\partial \Psi_2} & \dfrac{\partial S_2}{\partial \Psi_2} \end{pmatrix} \begin{pmatrix} \dfrac{\delta G}{\delta S_1} \\ \dfrac{\delta G}{\delta S_2} \end{pmatrix} \\
&= - \int d^3x \ \frac{\delta F}{\delta \mathbf{u}} \cdot \begin{pmatrix}\nabla\Psi_1 & \nabla\Psi_2\end{pmatrix} \begin{pmatrix} \dfrac{\partial S_1}{\partial \Psi_1} & \dfrac{\partial S_2}{\partial \Psi_1} \\ \dfrac{\partial S_1}{\partial \Psi_2} & \dfrac{\partial S_2}{\partial \Psi_2} \end{pmatrix} \begin{pmatrix} \dfrac{\delta G}{\delta S_1} \\ \dfrac{\delta G}{\delta S_2} \end{pmatrix} \\
&= - \int d^3x \ \frac{\delta F}{\delta \mathbf{u}} \cdot \begin{pmatrix}\nabla S_1 & \nabla S_2\end{pmatrix} \begin{pmatrix} \dfrac{\delta G}{\delta S_1} \\ \dfrac{\delta G}{\delta S_2} \end{pmatrix} \\
&= \int d^3x \ \begin{pmatrix}S_1 & S_2\end{pmatrix} \frac{\delta F}{\delta \mathbf{u}} \cdot \nabla \begin{pmatrix} \dfrac{\delta G}{\delta S_1} \\ \dfrac{\delta G}{\delta S_2} \end{pmatrix},
\end{aligned} \tag{5.3.20}$$

where we have integrated by parts and used the fact that $\nabla \cdot (\delta F/\delta \mathbf{u}) = 0$ by definition. A similar computation holds for the terms proportional to $\delta G/\delta \mathbf{u}$. Thus the Poisson bracket (5.3.15) retains the same form under the change of variables $(\mathbf{u}, \Psi_1, \Psi_2) \mapsto (\mathbf{u}, S_1, S_2)$. □

Let us apply this transformation to the active Hamiltonian (5.3.16). We have

$$H_a \mapsto H_a' = H_a + \int d^3x \ \frac{\kappa}{2} \log \left| \frac{\partial(S_1, S_2)}{\partial(\Psi_1, \Psi_2)}(\Psi_1, \Psi_2) \right|^2. \tag{5.3.21}$$

The additional term is a Casimir functional of the Poisson bracket (5.3.15), as it is of the form

$$C_g = \int d^3x \ g(\Psi_1, \Psi_2), \tag{5.3.22}$$

where g is an arbitrary real function of Ψ_1, Ψ_2 but not their spatial derivatives. Therefore, if F is a gauge-invariant, we have for all $s = (S_1, S_2) \in \mathrm{Diff}(\mathbb{R}^2)$ that

$$s^*\{F, H_a\} = \{s^*F, s^*H_a\} = \{F, H_a + C\} = \{F, H_a\}, \tag{5.3.23}$$

which shows that $X_{H_a} = \{\cdot, H_a\}$ maps gauge-invariant functionals to gauge-invariant functionals.

To summarise, for an unnormalised director field $\mathbf{B}$ that is divergence-free and admits a global Clebsch representation (5.3.10), the system (5.3.17a,b) is a noncanonical Hamiltonian system on $(\mathrm{Vect}_\mu(\mathbb{R}^3) \ltimes C^\infty(\mathbb{R}^3, \mathbb{R}^2))^*$. The group $\mathrm{Diff}(\mathbb{R}^2)$ of gauge transformations (5.3.18) acts by Poisson automorphisms on $(\mathrm{Vect}_\mu(\mathbb{R}^3) \ltimes C^\infty(\mathbb{R}^3, \mathbb{R}^2))^*$ and transforms the active Hamiltonian (5.3.16) by adding a Casimir functional $H_a \mapsto H_a + C$. The Hamiltonian vector field X_{H_a} is therefore gauge-invariant and induces a vector field on the quotient space

$$(\mathrm{Vect}_\mu(\mathbb{R}^3) \ltimes C^\infty(\mathbb{R}^3, \mathbb{R}^2))^* \to (\mathrm{Vect}_\mu(\mathbb{R}^3) \ltimes C^\infty(\mathbb{R}^3, \mathbb{R}^2))^* / \mathrm{Diff}(\mathbb{R}^2), \tag{5.3.24}$$

even though H_a is not a pullback of some effective Hamiltonian on the quotient space.

Remark 5.2. In ordinary MHD, only gauge transformations with $\partial(S_1, S_2)/\partial(\Psi_1, \Psi_2) = 1$ are allowed, as both the magnitude and direction of $\mathbf{B}$ need to be kept constant. The appropriate gauge group in this case is the group $\mathrm{Diff}_\mu(\mathbb{R}^2)$ of volume-preserving diffeomorphisms, and any Hamiltonian that depends on the Clebsch potentials through $\mathbf{B} = \nabla\Psi_1 \times \nabla\Psi_2$ will factor through the quotient map.

There is an analogous construction in two dimensions, where we have a single Clebsch potential Ψ and $\mathbf{B} = \nabla_\times \Psi$, as in section **5.3.2**. The Poisson bracket in this case is

$$\begin{aligned}\{F, G\} = -\int d^2x\, \mathbf{u} \cdot \left(\frac{\delta F}{\delta \mathbf{u}} \cdot \nabla \frac{\delta G}{\delta \mathbf{u}} - \frac{\delta G}{\delta \mathbf{u}} \cdot \nabla \frac{\delta F}{\delta \mathbf{u}} \right) \\ + \Psi \left(\frac{\delta F}{\delta \mathbf{u}} \cdot \nabla \frac{\delta G}{\delta \Psi} - \frac{\delta G}{\delta \mathbf{u}} \cdot \nabla \frac{\delta F}{\delta \Psi} \right),\end{aligned} \tag{5.3.25}$$

which is the $(-)$-Lie–Poisson bracket on the dual of the semidirect product Lie algebra $\mathrm{Vect}_\mu(\mathbb{R}^2) \ltimes C^\infty(\mathbb{R}^2)$. The active Hamiltonian is

$$H_a[\mathbf{u}, \Psi] = \int d^2x\, \frac{\kappa}{2} \log |\nabla\Psi|^2, \tag{5.3.26}$$

and the gauge transformation is a diffeomorphism $S : \mathbb{R} \to \mathbb{R}$, taking Ψ to $S(\Psi)$. The group $\mathrm{Diff}(\mathbb{R})$ of gauge transformations also acts on $(\mathrm{Vect}_\mu(\mathbb{R}^2) \ltimes C^\infty(\mathbb{R}^2))^*$ by Poisson automorphisms, which can be verified by a similar computation to (5.3.20). The active Hamiltonian transforms under this gauge transformation as

$$H_a \mapsto H_a' = H_a + \int d^2x\, \frac{\kappa}{2} \log \left| \frac{dS}{d\Psi}(\Psi) \right|^2, \tag{5.3.27}$$

gaining an additional term that is a Casimir functional of the Poisson bracket (5.3.25), therefore leaving the time evolution operator X_{H_a} gauge invariant.

5.4 Waves in the active rod system

In this section we study the wave solutions of the active rod system (5.2.6a,b). We begin by considering linear waves, then we make use of the *energy-momentum method* to study nonlinear waves using a variational principle. For contractile ($\kappa > 0$) rods, we show that the active rod system (5.2.6a,b) admit *Alfvén wave* solutions [2, 3, 22, 169, 194].

5.4.1 Linear waves

Let us consider infinitesimal perturbations about the static constant-field equilibrium, so that $\mathbf{u} = \delta\mathbf{u}$, $\mathbf{B} = \mathbf{e}_z + \delta\mathbf{B}$. A pressure perturbation $P = P_0 + \delta P$ will also be generated. The active rod system (5.2.6a,b) linearises to

$$\partial_t \delta\mathbf{u} = -\nabla\delta P + \kappa\left(\mathbf{e}_z \cdot \nabla\delta\mathbf{B} + (\nabla\cdot\delta\mathbf{B})\,\mathbf{e}_z - 2\mathbf{e}_z\mathbf{e}_z\mathbf{e}_z : \nabla\delta\mathbf{B}\right), \quad \nabla\cdot\delta\mathbf{u} = 0, \tag{5.4.1a}$$

$$\partial_t \delta\mathbf{B} = \mathbf{e}_z \cdot \nabla\delta\mathbf{u}. \tag{5.4.1b}$$

We look for plane wave solutions $\delta\mathbf{u}, \delta\mathbf{B} \propto \exp(-\mathrm{i}\omega t + \mathrm{i}\mathbf{k}\cdot\mathbf{x})$. We decompose the wavenumber $\mathbf{k}$ as $\mathbf{k} = \mathbf{k}_\perp + k_z\mathbf{e}_z$, where $\mathbf{k}_\perp$ is perpendicular to the z-axis, and similarly for $\delta\mathbf{u}$ and $\delta\mathbf{B}$. The system (5.4.1a,b) then becomes

$$-\omega\delta\mathbf{u} = -\mathbf{k}\delta P + \kappa\left(k_z\delta\mathbf{B} + \mathbf{k}\cdot\delta\mathbf{B}\mathbf{e}_z - 2k_z\delta B_z\mathbf{e}_z\right), \quad \mathbf{k}\cdot\delta\mathbf{u} = 0, \tag{5.4.2a}$$

$$-\omega\delta\mathbf{B} = k_z\delta\mathbf{u}. \tag{5.4.2b}$$

Taking $\mathbf{k}\cdot$ (5.4.2a) gives an expression for δP:

$$\delta P = \frac{2\kappa k_z \mathbf{k}_\perp\cdot\delta\mathbf{B}}{|\mathbf{k}|^2}. \tag{5.4.3}$$

There are no waves in the system (5.4.2a,b) with $k_z = 0$. Thus we can, without loss of generality, consider wavenumbers $\mathbf{k}$ with $k_z \neq 0$. As $\mathbf{k}$ is in general position with the z-axis, the components of $\delta\mathbf{u}_\perp$ are good coordinates for the plane $\mathbf{k}\cdot\delta\mathbf{u} = 0$. The equation (5.4.2b) implies that $\delta\mathbf{B}$ is parallel to $\delta\mathbf{u}$, and in particular $\mathbf{k}\cdot\delta\mathbf{B} = 0$ using (5.4.2a), so the unnormalised director field $\mathbf{B}$ is divergence-free. The system (5.4.2a,b) can be simplified as

$$\omega^2\delta\mathbf{u}_\perp = \kappa k_z^2\left(\mathbf{I} - \frac{2\mathbf{k}_\perp\mathbf{k}_\perp}{|\mathbf{k}|^2}\right)\cdot\delta\mathbf{u}_\perp. \tag{5.4.4}$$

The four branches of the dispersion relation can then be immediately read off from (5.4.4):

$$\omega_a^2 = \kappa k_z^2, \qquad \delta\mathbf{u}_\perp \perp \mathbf{k}_\perp, \tag{5.4.5a}$$

$$\omega_s^2 = \kappa k_z^2\left(1 - \frac{2|\mathbf{k}_\perp|^2}{|\mathbf{k}|^2}\right), \qquad \delta\mathbf{u}_\perp \parallel \mathbf{k}_\perp. \tag{5.4.5b}$$

For contractile active rods, where $\kappa > 0$, the first mode (5.4.5a) corresponds to the *shear-Alfvén wave* in MHD, and the second mode (5.4.5b) corresponds to what remains of the *slow magnetosonic wave* in MHD in the incompressible limit. Alfvén waves were first identified in 1942 as a mechanism for energy transport in the solar wind [3]. For a modern account of waves in MHD, see e.g. [22, 169].

A crucial difference between the active rod system and MHD is that the "slow wave" in the active rod system has an extra factor of 2 in the dispersion relation compared to that of incompressible MHD, so it is in fact unstable when

$$\cos^2\theta = \frac{k_z^2}{|\mathbf{k}|^2} < \frac{\sqrt{2}}{2}, \tag{5.4.6}$$

or equivalently when the angle θ between $\mathbf{k}$ and the z-axis i.e. the background field direction is larger than $\pi/4$. This instability is discussed in [162]. The stability property reverses for extensile active rods, where $\kappa < 0$.

The linearised active rod system (5.4.1a,b) conserves the following quadratic invariant:

$$\mathcal{Q} = \frac{1}{2}|\delta\mathbf{u}|^2 + \frac{\kappa}{2}\delta\mathbf{B}\cdot(\mathbf{I} - 2\mathbf{e}_z\mathbf{e}_z)\cdot\delta\mathbf{B}. \tag{5.4.7}$$

Indeed,

$$\partial_t\mathcal{Q} = -\nabla\cdot\left(\delta P\delta\mathbf{u} + \mathbf{e}_z\delta\mathbf{u}\cdot(\mathbf{I} - 2\mathbf{e}_z\mathbf{e}_z)\cdot\delta\mathbf{B}\right). \tag{5.4.8}$$

The quantity $\mathcal{Q}$ is closely related to the available energy for the static constant-field equilibrium (see section **2.4.2**, in particular (2.4.12)). Indeed, the static constant-field equilibrium $\mathbf{u}_e = 0, \mathbf{B}_e = \mathbf{e}_z$ is the critical point of the available energy functional functional .

$$A_0[\mathbf{u},\mathbf{B}] = H_a[\mathbf{u},\mathbf{B}] - \kappa\int d^3x\ \mathbf{B}\cdot\mathbf{e}_z, \tag{5.4.9}$$

where H_a is as in (5.3.3), and the integral $\int d^3x\ \mathbf{B}\cdot\mathbf{e}_z$ is a Casimir functional of the Poisson bracket (5.3.1) with $\nabla\cdot\mathbf{B} = 0$ required. Expanding A_0 (5.4.9) around the constant-field equilibrium gives

$$\begin{aligned} A_0\left[\delta\mathbf{u}, \mathbf{e}_z + \delta\mathbf{B}\right] &= \int d^3x\ \left(\frac{1}{2}|\delta\mathbf{u}|^2 + \frac{\kappa}{2}\delta\mathbf{B}\cdot(\mathbf{I} - 2\mathbf{e}_z\mathbf{e}_z)\cdot\delta\mathbf{B} + O\left(\delta\mathbf{B}^3\right)\right) \\ &= \int d^3x\ \mathcal{Q} + O\left(\delta\mathbf{B}^3\right), \end{aligned} \tag{5.4.10}$$

where $\mathcal{Q}$ is as in (5.4.7). Thus A_0 (5.4.9) is the appropriate nonlinear extension of the invariant $\int d^3x\ \mathcal{Q}$ of the linearised equations (5.4.1a,b).

5.4.2 Finite-amplitude waves in contractile rods

We have so far considered Alfvén waves in the active rod suspension as infinitesimal perturbations to a straight field background. For contractile ($\kappa > 0$) rods, the active rod suspension supports *finite-amplitude* Alfvén waves. Finite-amplitude Alfvén waves can be found in the ideal MHD equations and their various extensions [2, 194], and they are closely related to the *cross helicity* Casimir functional (2.6.40). We require $\nabla \cdot \mathbf{B} = 0$ in the following.

To find finite-amplitude (i.e. fully nonlinear) travelling wave solutions, we need the *energy-momentum method* (see section **2.4.2**, in particular (2.4.18)), where we consider travelling wave solutions as the critical points of augmented available energy functionals $A = H + C - J$, where J is a non-Casimir conserved quantity. These critical points will evolve in time according to $\partial_t = X_H = X_J$. For travelling waves, J should be taken as the momentum of the fluid along a fixed direction:

$$J = \int d^3x \; \mathbf{u}_0 \cdot \mathbf{u}, \tag{5.4.11}$$

where $\mathbf{u}_0$ is a constant vector field. One easily checks that $\{J, H_a\} = 0$. The Hamiltonian flow X_J of J is (using (5.3.2a,b))

$$\partial_\epsilon \mathbf{u} = -\mathbf{u}_0 \cdot \nabla \mathbf{u}, \qquad \partial_\epsilon \mathbf{B} = -\mathbf{u}_0 \cdot \nabla \mathbf{B}, \tag{5.4.12}$$

where ϵ is the flow parameter. So the flow of X_J is uniform translation in space, as expected. A particularly interesting class of finite-amplitude waves can be obtained from the critical points of the following augmented available energy functional:

$$A_\lambda^{(w)} = H_a - \lambda \int d^3x \; (\mathbf{u} - \mathbf{u}_0) \cdot \mathbf{B} - J, \tag{5.4.13}$$

where λ is a real number, H_a is as in (5.3.3) and J is as in (5.4.11). The term pre-multiplied by λ is a linear combination of the Casimir $\int d^3x \; \mathbf{u}_0 \cdot \mathbf{B}$ and the *cross helicity* Casimir $\int d^3x \; \mathbf{u} \cdot \mathbf{B}$ (2.6.40). Critical points $\mathbf{u}_w, \mathbf{B}_w$ of $A_\lambda^{(w)}$ (5.4.13) satisfy the equations

$$\mathbf{u}_w - \mathbf{u}_0 - \lambda \mathbf{B}_w = 0, \tag{5.4.14a}$$

$$\kappa \frac{\mathbf{B}_w}{|\mathbf{B}_w|^2} - \lambda \, (\mathbf{u}_w - \mathbf{u}_0) = 0, \tag{5.4.14b}$$

which leads to the following conditions

$$|\mathbf{B}_w|^2 = \frac{\kappa}{\lambda^2}, \quad \nabla \cdot \mathbf{B}_w = 0, \quad \mathbf{u}_w - \mathbf{u}_0 = \lambda \mathbf{B}_w. \tag{5.4.15}$$

There is no solution to (5.4.15) when the active rods are extensile ($\kappa < 0$). For contractile ($\kappa > 0$) rods, any divergence-free $\mathbf{B}_w$ with constant norm is a solution for (5.4.15). In the following we take $\kappa = 1$ and $\lambda = \pm 1$, as the other solutions can be obtained by rescaling $\mathbf{B}_w$ and $\mathbf{u}_w - \mathbf{u}_0$. We can also state (5.4.15) in terms of the shifted *Elsässer variables* $\boldsymbol{\zeta}_\pm = (\mathbf{u}_w - \mathbf{u}_0) \pm \mathbf{B}_w$ [22, 59]:

$$\boldsymbol{\zeta}_\mp = 0, \qquad |\boldsymbol{\zeta}_\pm| = \sqrt{2}, \qquad \nabla \cdot \boldsymbol{\zeta}_\pm = 0. \tag{5.4.16}$$

An example of such finite-amplitude waves is where $\mathbf{u}_0 = -\lambda \mathbf{e}_z$ and $\mathbf{B}_w$ is

$$\mathbf{B}_w(x, y, z, t) = (\sin\theta_z \cos k_z(z + \lambda t), \sin\theta_z \sin k_z(z + \lambda t), \cos\theta_z)\,, \tag{5.4.17}$$

where k_z and θ_z are constants. Expanding (5.4.17) for $\theta_z \ll 1$ gives

$$\mathbf{B}_w = \mathbf{e}_z + \theta_z \delta\mathbf{B} + O(\theta_z^2), \tag{5.4.18a}$$

$$\mathbf{u}_w = \theta_z \delta\mathbf{u} + O(\theta_z^2), \tag{5.4.18b}$$

where $\delta\mathbf{u}, \delta\mathbf{B}$ are the shear-Alfvén waves (5.4.5a) found in section **5.4.1** with $\omega_a = -\lambda k_z$. In light of this example, we call the solutions of (5.4.15) *finite-amplitude Alfvén waves*, as they are travelling wave solutions to the fully nonlinear active rod system (5.2.6a,b) that can be thought of as nonlinear generalisations of the shear-Alfvén waves in the linearised equations (5.4.1a,b).

Remark 5.3. It is also possible to obtain finite-amplitude travelling wave solutions by first obtaining the static solutions $\mathbf{u}_e, \mathbf{B}_e$ with the energy-Casimir method for the available energy $A_\lambda^{(w)}$ (5.4.13) with $\mathbf{u}_0 = 0$, then applying a Galilean frame transformation to $\mathbf{u}_e, \mathbf{B}_e$ [2, 194]. We prefer the energy-momentum method because it incorporates the Galilean boost automatically through the inclusion of the momentum functional J.

5.5 Static force-free equilibrium of the active rod system

In this section we analyse static ($\mathbf{u} = 0$), steady state ($\partial_t = 0$) solutions of the active rod system (5.2.6a,b). The unnormalised director field $\mathbf{B}$ then satisfies

$$-\nabla P + \kappa \nabla \cdot \frac{\mathbf{B}\mathbf{B}}{|\mathbf{B}|^2} = 0. \tag{5.5.1}$$

Taking $\mathbf{B}\cdot$ (5.5.1) and rearranging gives

$$\mathbf{B} \cdot \nabla \left(-P + \frac{\kappa}{2} \log|\mathbf{B}|^2 \right) + \kappa \nabla \cdot \mathbf{B} = 0, \tag{5.5.2}$$

so we can gauge-fix the magnitude degree of freedom as $|\mathbf{B}| = \exp(-P/\kappa)$ to obtain a divergence-free $\mathbf{B}$. Under this choice, equation (5.5.1) becomes

$$\mathbf{B} \times \nabla \times \frac{\mathbf{B}}{|\mathbf{B}|^2} = 0, \qquad \nabla \cdot \mathbf{B} = 0. \tag{5.5.3}$$

The configuration described by (5.5.3) is called a *force-free field* in MHD [169]. Using the language of section **5.2.2**, equation (5.5.3) can be written as

$$\mathbf{J}_f \times \mathbf{B} = 0, \quad \text{where } \mathbf{J}_f = \nabla \times \mathbf{H} \quad \text{and} \quad \mathbf{H} = \kappa \frac{\mathbf{B}}{|\mathbf{B}|^2}, \tag{5.5.4}$$

corresponding to a configuration where the Lorentz force (5.2.11) on the fluid vanishes. An equivalent way to express (5.5.3) is

$$\nabla \times \frac{\mathbf{B}}{|\mathbf{B}|^2} = \alpha(\mathbf{x})\mathbf{B}, \qquad \mathbf{B} \cdot \nabla \alpha(\mathbf{x}) = 0. \tag{5.5.5}$$

where $\alpha(\mathbf{x})$ is some scalar field. The requirement $\mathbf{B} \cdot \nabla \alpha = 0$, which is derived from taking the divergence of (5.5.5) and setting $\nabla \cdot \mathbf{B} = 0$, means that α is constant along the field lines of $\mathbf{B}$. As an example, we can take α to be a constant. Then $\mathbf{B}$ becomes what is called a *linear force-free field*:

$$\nabla \times \frac{\mathbf{B}}{|\mathbf{B}|^2} = \alpha \mathbf{B}. \tag{5.5.6}$$

One possible scenario when α is required to be a constant is when the field lines are "chaotic", in the sense that any two field lines can get indefinitely close to each other. In such a configuration, $\alpha(\mathbf{x})$ must also be constant across field lines if it is continuous. As $\alpha(\mathbf{x})$ is both constant along and across field lines, it cannot vary with $\mathbf{x}$ i.e. is a constant.

The solutions to (5.5.6) are in fact critical points of the following available energy functional:

$$A_T\left[\mathbf{u}, \mathbf{B}\right] = H_a\left[\mathbf{u}, \mathbf{B}\right] - \frac{\kappa\alpha}{2} \int d^3x \; \mathbf{A} \cdot \mathbf{B}, \tag{5.5.7}$$

where H_a is as in (5.3.3) and the extra term is the *magnetic helicity* of $\mathbf{B}$ (2.6.37), which is a Casimir functional of the Poisson bracket (5.3.1) when $\nabla \cdot \mathbf{B} = 0$. Indeed, taking the functional derivatives of A_T (5.5.7) gives

$$\frac{\delta A_T}{\delta \mathbf{u}} = \mathbf{u}, \tag{5.5.8a}$$

$$\frac{\delta A_T}{\delta \mathbf{B}} = \kappa \left(\frac{\mathbf{B}}{|\mathbf{B}|^2} - \alpha \mathbf{A} \right), \tag{5.5.8b}$$

from which we recover (5.5.6) and $\mathbf{u} = 0$ as the critical points of A_T (5.5.7). This variational principle is the analogue of *Taylor relaxation* [173] for MHD in a nonlinear medium, where the linear force-free fields are obtained from minimising the energy subject to helicity conservation.

Another case where the force-free condition (5.5.3) admits further simplification is when the unnormalised director field admits a global Clebsch representation $\mathbf{B} = \nabla\Psi_1 \times \nabla\Psi_2$ (see section **5.3.2**). Any quantity $\alpha(\mathbf{x})$ constant along the field lines is then expressible as a function of the Clebsch potentials: $\alpha = \alpha(\Psi_1, \Psi_2)$. Taking the dot products of (5.5.5) with $\nabla\Psi_1, \nabla\Psi_2$ yields the following equations for the Clebsch potentials

$$\nabla\Psi_1 \cdot \nabla \times \frac{\nabla\Psi_1 \times \nabla\Psi_2}{|\nabla\Psi_1 \times \nabla\Psi_2|^2} = 0, \qquad \nabla\Psi_2 \cdot \nabla \times \frac{\nabla\Psi_1 \times \nabla\Psi_2}{|\nabla\Psi_1 \times \nabla\Psi_2|^2} = 0. \tag{5.5.9}$$

The solutions of (5.5.9) are the critical points of the active Hamiltonian H_a (5.3.16) in the Clebsch formulation. Indeed, for $(i, j) = (1, 2)$ or $(2, 1)$, the functional derivatives of H_a (5.3.16) are

$$\frac{\delta H_a}{\delta \mathbf{u}} = \mathbf{u}, \tag{5.5.10a}$$

$$\frac{\delta H_a}{\delta \Psi_i} = (-1)^j \kappa \nabla \cdot \frac{\nabla\Psi_j \times (\nabla\Psi_1 \times \nabla\Psi_2)}{|\nabla\Psi_1 \times \nabla\Psi_2|^2}, \tag{5.5.10b}$$

from which we recover (5.5.9) and $\mathbf{u} = 0$ as the critical points of H_a (5.3.16). The variational principle (5.5.10b) is the nonlinear medium analogue for the Clebsch potential variational principle for force-free fields in ordinary MHD [151, 191].

5.6 Conclusion

In this chapter we have studied the active rod system (5.2.6a,b) in analogy with MHD. The active rod system (5.2.6a,b) can be formulated as a MHD system in an electromagnetically nonlinear medium (5.2.8, 5.2.13) [113, 158] (section **5.2.2**). It also shares the noncanonical Hamiltonian structure with incompressible MHD (5.3.1) [6, 94, 138], with a magnetic energy density of $(\kappa/2)\log(|\mathbf{B}|^2)$ instead of $|\mathbf{B}|^2/2$ (section **5.3.1**). The main difference between the active rod system and MHD is that, for the active rods, the magnitude $|\mathbf{B}|$ is a spurious degree of freedom that can be removed, while in MHD the divergence-free condition $\nabla \cdot \mathbf{B}$ removes a different degree of freedom.

The Clebsch potential formulation $\mathbf{B} = \nabla\Psi_1 \times \nabla\Psi_2$ [133, 169] provides a middle ground that accommodates both conditions – the divergence-free condition is always met, and certain rescaling transformations of $\mathbf{B}$ become gauge transformations in the corresponding Hamiltonian formulation (sections **5.3.2**, **5.3.3**). In the Clebsch potential formulation,

the gauge transformations are Poisson automorphisms, and the Hamiltonian functional transform as $H_a \mapsto H_a + C$ for some Casimir functional C, so the Hamiltonian vector field X_{H_a} is gauge-invariant and induces a vector field on the quotient.

We have also studied the equilibrium solutions and waves of the active rod system (5.2.6a,b). For contractile ($\kappa > 0$) rods, we discovered that the active rod system admits both linear and nonlinear *Alfvén waves* (section **5.4**), a property ubiquitous to MHD and its various extensions [2, 3, 22, 169, 194]. The linear waves conserve a quadratic invariant $\mathfrak{Q}$ that corresponds to the available energy of the static constant-field equilibrium (section **5.4.1**), while the finite-amplitude Alfvén waves can be found from a different variational principle using the energy-momentum method (section **5.4.2**). We also studied the static force-free equilibrium of the active rod system (5.5.1). These equilibria correspond to the force-free fields in MHD, which can be obtained from variational principles [151, 173, 191], and we obtained their active rod analogues (section **5.5**).

We remark that the $\mathbf{Q}$-tensor formulation is far more common in the active swimmers literature than the director formulation using $\mathbf{n}$ or $\mathbf{B}$ discussed in this chapter [52, 53, 75, 90, 115, 121, 147, 174, 175]. In this formulation one takes a symmetric rank-2 tensor $\mathbf{Q} = \langle \mathbf{nn} \rangle$, which represents some statistical average of the dyadic product of $\mathbf{n}$ with itself, as the internal state variable[3]. For rod-like swimmers, the $\mathbf{Q}$-tensor evolves in time as

$$\partial_t \mathbf{Q} + \mathbf{u} \cdot \nabla \mathbf{Q} - (\nabla \mathbf{u})^T \cdot \mathbf{Q} - \mathbf{Q} \cdot \nabla \mathbf{u} + 2\mathrm{Tr}(\mathbf{Q} \cdot \mathbf{E})\mathbf{Q} = \mathbf{R}[\mathbf{Q}], \tag{5.6.1}$$

where $\mathbf{R}[\mathbf{Q}]$ contains relaxation terms due to liquid crystal effects. Ignoring these relaxation effects, we can rewrite (5.6.1) in terms of an unnormalised *conformation tensor* $\mathbf{C}$. We require that $\mathbf{C}$ evolves in time by the upper-convected derivative, or the Lie derivative of symmetric rank-$(2,0)$ tensors[4]:

$$\partial_t \mathbf{C} + \mathbf{u} \cdot \nabla \mathbf{C} - (\nabla \mathbf{u})^T \cdot \mathbf{C} - \mathbf{C} \cdot \nabla \mathbf{u} = 0, \tag{5.6.2}$$

from which taking $\mathbf{Q} = \mathbf{C}/\mathrm{Tr}(\mathbf{C})$ recovers (5.6.1) with $\mathbf{R} = 0$. We can attempt to formulate the dynamics of $(\mathbf{u}, \mathbf{C})$ as a noncanonical Hamiltonian system on the dual of the semidirect product Lie algebra $\mathrm{Vect}_\mu(\mathbb{R}^3) \ltimes \Gamma(S^2 T^* \mathbb{R}^3)$. The Poisson bracket is [16, 17, 57, 127, 128]

$$\begin{aligned} \{F, G\} = -\int d^3x \, \mathbf{u} \cdot \left(\frac{\delta F}{\delta \mathbf{u}} \cdot \nabla \frac{\delta G}{\delta \mathbf{u}} - \frac{\delta G}{\delta \mathbf{u}} \cdot \nabla \frac{\delta F}{\delta \mathbf{u}} \right) \\ + \mathrm{Tr}\left(\mathbf{C} \cdot \left(\pounds_{\frac{\delta F}{\delta \mathbf{u}}} \frac{\delta G}{\delta \mathbf{C}} - \pounds_{\frac{\delta G}{\delta \mathbf{u}}} \frac{\delta F}{\delta \mathbf{C}} \right) \right), \end{aligned} \tag{5.6.3}$$

[3]The convention on the normalisation of $\mathrm{Tr}\mathbf{Q}$ varies. Some authors subtract multiples of $\mathbf{I}$ from the definition of $\mathbf{Q}$ to make it traceless.

[4]We do not make the distinction between tensors and tensor densities because we only work with incompressible vector fields $\nabla \cdot \mathbf{v} = 0$.

which $\mathcal{L}_{\mathbf{v}}\mathbf{D}$ in (5.6.3) is the lower convected derivative, or the Lie derivative of symmetric rank-$(0,2)$ tensors (cf. section **2.3.2**):

$$\mathcal{L}_{\mathbf{v}}\mathbf{D} = \mathbf{v}\cdot\nabla\mathbf{C} + (\nabla\mathbf{v})\cdot\mathbf{D} + \mathbf{C}\cdot(\nabla\mathbf{v})^T. \tag{5.6.4}$$

Choosing the Hamiltonian $H_a[\mathbf{u},\mathbf{C}] = \int d^3x\ (|\mathbf{u}|^2/2 + h(\mathbf{C}))$ recovers (5.6.2) and the momentum equation for an incompressible fluid where the stress is

$$\boldsymbol{\sigma} = \mathbf{C}\cdot\frac{\partial h}{\partial\mathbf{C}} + \frac{\partial h}{\partial\mathbf{C}}\cdot\mathbf{C}, \tag{5.6.5}$$

ignoring the trace contribution as it is absorbed in the pressure P. If we choose

$$h(\mathbf{C}) = \frac{\kappa}{2}\log\left(\mathrm{Tr}\mathbf{C}\right), \tag{5.6.6}$$

we recover the active stress most commonly used in the active swimmers literature [52, 53, 75, 90, 115, 121, 147, 174, 175]:

$$\boldsymbol{\sigma} = \frac{\kappa\mathbf{C}}{\mathrm{Tr}\mathbf{C}} = \kappa\mathbf{Q}. \tag{5.6.7}$$

Repeating the argument in section **5.3.1**, we see that the maps $\mathbf{C}(\mathbf{x},t)\mapsto \mathrm{e}^{\mathcal{B}(\mathbf{x})}\mathbf{C}(\mathbf{x},t)$ are gauge transformations, and the Hamiltonian vector field X_{H_a} can be pushed down to the quotient space for the normalised $\mathbf{Q}$-tensor formulation $(\mathbf{u},\mathbf{Q})$.

We can thus think of the $\mathbf{Q}$-tensor formulation as a Hamiltonian system for the unnormalised conformation tensor $\mathbf{C}$, with its magnitude being a gauge degree of freedom. On paper, such a $\mathbf{Q}$-tensor formulation would be a generalisation of the director formulation, as it can handle more complicated geometries where $\mathbf{Q}$ is not a pure dyadic product $\mathbf{nn}$, most notably defect geometries where $\mathbf{n}$ is ill-defined[5] [34, 67, 75, 121].

However, as far as the author is aware, the $\mathbf{Q}$-tensor formulation has considerably fewer interesting structural properties. In particular, there is no corresponding condition to $\nabla\cdot\mathbf{B}=0$ for the conformation tensor $\mathbf{C}$, so the Clebsch potential formulation discussed in section **5.3.2** does not carry over, and there is no finer description to the gauge transformation than simply a time-independent change in magnitude by a scalar field. Moreover, the cross helicity (2.6.40) and magnetic helicity (2.6.37) Casimirs have no obvious analogues, so the nonlinear Alfvén waves (section **5.4.2**) and the static force-free field solutions (section **5.5**) do not carry over to the $\mathbf{Q}$-tensor formulation. Further comparative study is needed for the similarities and differences between the director formulation and the $\mathbf{Q}$-tensor formulation.

[5]Defect geometries can be modelled by the Clebsch potential formulation (section **5.3.2**), but the global existence of Clebsch potentials is always rife with problems [133, 155, 193]. A possible remedy in two dimensions is to lift the Clebsch potentials to a branched cover by a Riemann surface (see e.g. [65]). This introduces considerable complications to the theory but could be a worthwhile direction for future investigation.

Appendix A

Complete lifts, vector bundle structures and metrics on $T^{(N)}M$

This appendix details some geometric constructions on the higher order tangent bundle $T^{(N)}M$ introduced in chapter **3**. The sections in this appendix are based on the author's work [41] on multibead-chain suspensions. We will assume some familiarity with vector bundles and Riemannian geometry (see e.g. [100, 179]). The main references are [49, 50, 109, 192].

A.1 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 $u \in \mathrm{Vect}(M)$ to $u^{\#} \in \mathrm{Vect}(T^{(N)}M)$ (3.2.8,3.3.7). For more details, see [109, 192].

Let M be a manifold. Recall that a *diffeomorphism* $\varphi : M \to M$ is a smooth bijective map from M to M with a smooth inverse. In local coordinates, a diffeomorphism φ is an invertible coordinate transformation $x^i \mapsto \varphi^i(x)$. The collection of diffeomorphisms of a manifold M is denoted by $\mathrm{Diff}(M)$, which can be thought of as an infinite-dimensional Lie group [56, 107].

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

$$\varphi^{\#} : \alpha(t) \mapsto (\varphi \circ \alpha)(t). \tag{A.1.1}$$

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

$$(\varphi \circ \psi)^{\#}(\alpha) = \varphi^{\#}\left(\psi^{\#}(\alpha)\right) = (\varphi \circ \psi \circ \alpha)(t). \tag{A.1.2}$$

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

$$\alpha(t) \overset{(N)}{\sim} \beta(t) \Leftrightarrow \alpha(0) = \beta(0), \frac{d^a}{dt^a}\alpha(t)\bigg|_{t=0} = \frac{d^a}{dt^a}\beta(t)\bigg|_{t=0} \text{ for } a = 1, \cdots, N. \quad \text{(A.1.3)}$$

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

$$\alpha^i(t) = x^i + \sum_{a=1}^{N} y^i_{(a)} \frac{t^a}{a!} + O(t^{N+1}). \quad \text{(A.1.4)}$$

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

$$\left(\varphi^{\#}(\alpha)\right)^i(t) = \varphi^i(\alpha(t)) = \varphi^i(\alpha(0)) + \sum_{a=1}^{N} \frac{t^a}{a!}\left(\frac{d^a}{dt^a}\varphi^i(\alpha(t))\bigg|_{t=0}\right) + O(t^{N+1}). \quad \text{(A.1.5)}$$

Note that

$$\frac{d^a}{dt^a}\varphi^i\left(x^i + \sum_{a=1}^{N} y^i_{(a)}\frac{t^a}{a!} + O(t^{N+1})\right)\bigg|_{t=0} \quad \text{(A.1.6)}$$

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 $\overset{(N)}{\sim}$, 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

$$\varphi \in \mathrm{Diff}(M) \mapsto \varphi^{\#} \in \mathrm{Diff}(T^{(N)}M), \quad \text{(A.1.7)}$$

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

$$\varphi^i(x) = x^i + su^i(x) + O(s^2), \quad \text{(A.1.8a)}$$

$$\psi^i(x) = x^i + rv^i(x) + O(r^2), \quad \text{(A.1.8b)}$$

and comparing the two sides of the expression

$$\frac{\partial^2}{\partial s \partial r}\bigg|_{s=0,r=0} \left(\varphi \circ \psi \circ \varphi^{-1}\right)^{\#} = \frac{\partial^2}{\partial s \partial r}\bigg|_{s=0,r=0} \left(\varphi^{\#} \circ \psi^{\#} \circ \left(\varphi^{-1}\right)^{\#}\right), \quad \text{(A.1.9)}$$

we obtain a homomorphism of Lie algebras

$$u \in \mathrm{Vect}(M) \mapsto u^{\#} \in \mathrm{Vect}\left(T^{(N)}M\right), \quad \text{(A.1.10)}$$

which is precisely the complete lift given in (3.3.7).

A.2 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 $(x^i, y^i_{(a)})$ on $T^{(N)}M$, where the fibre coordinates $y^i_{(a)},\ a = 1, \cdots, N$ 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 $(x^i, y^i_{(a)}) \mapsto (\tilde{x}^i, \tilde{y}^i_{(a)})$ is not linear for $a \geq 2$. For example,

$$\tilde{y}^i_{(2)} = \frac{\partial \tilde{x}^i}{\partial x^j} y^j_{(2)} + \frac{\partial^2 \tilde{x}^i}{\partial x^j \partial x^k} y^j_{(1)} y^k_{(1)}. \tag{A.2.1}$$

(See appendix **A.1**.) In particular, the fibre coordinates do not transform like vectors under an arbitrary coordinate transformation.

In chapter **3**, we have considered considered moments of the distribution function $\psi(x, y_{(1)}, \ldots, y_{(N)})$ of the form

$$\int d\Gamma\ y^i_{(a)} \psi(x, y) \quad \text{for } a \geq 2 \text{ (say)}, \tag{A.2.2}$$

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 $(x^i, y^i_{(a)}) \mapsto (\tilde{x}^i, \tilde{y}^i_{(a)})$ 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 $(T \oplus \cdots \oplus T)M$ (N times) with the help of a *metric*, or more generally a *connection* on the tangent bundle [49, 50]. Given a metric g on M, we can consider its *Levi-Civita connection*[1] ∇, which 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

$$\nabla_X Y = X^j \left(\frac{\partial Y^i}{\partial x^j} + \Gamma^i_{jk} Y^k \right) \frac{\partial}{\partial x^i}, \tag{A.2.3}$$

where Γ^i_{jk} are the usual *Christoffel symbols* of the connection:

$$\nabla_{\frac{\partial}{\partial x^j}} \frac{\partial}{\partial x^k} = \Gamma^i_{jk} \frac{\partial}{\partial x^i}. \tag{A.2.4}$$

[1]The Levi-Civita connection is also known as the *Riemannian connection*.

An explicit formula for the Levi-Civita connection in terms of the metric tensor g_{ij} and its inverse g^{ij} is

$$\Gamma^i_{jk} = \frac{1}{2} g^{il} \left(\frac{\partial g_{lj}}{\partial x^k} + \frac{\partial g_{lk}}{\partial x^j} - \frac{\partial g_{jk}}{\partial x^l} \right). \tag{A.2.5}$$

The following construction works for any connection on TM. General connections are considered in appendix **A.3**. 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

$$\frac{Dw}{dt}(t) = \nabla_{v(t)} W\left(\alpha(t)\right). \tag{A.2.6}$$

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:

$$\left(\frac{Dw}{dt}\right)^i = \frac{\partial w^i}{\partial t} + \Gamma^i_{jk} v^j(t) w^k(t). \tag{A.2.7}$$

The components $(Dw/dt)^i$ transform like a vector under a change of coordinates, as long as the Christoffel symbols Γ^i_{jk} 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 $v(0), Dv/dt(0), \cdots, (D^{N-1}v/dt^{N-1})(0)$ evaluated at $t = 0$, which are genuine tangent vectors at $\alpha(0)$. This produces an isomorphism from $T^{(N)}M$ to $(T \oplus \cdots \oplus T)M$ (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

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

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

$$v^i(t) = y^i_{(1)} + \sum_{a=1}^{N-1} y^i_{(a)} \frac{t^a}{a!} + O(t^N). \tag{A.2.8}$$

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

$$\begin{aligned} v(0)^i &= y^i_{(1)}, \\ \left(\frac{Dv}{dt}(0)\right)^i &= y^i_{(2)} + \Gamma^i_{jk} y^j_{(1)} y^k_{(1)}, \\ \left(\frac{D^2v}{dt^2}(0)\right)^i &= y^i_{(3)} + \Gamma^i_{jk} y^j_{(1)} \left(y^k_{(2)} + \Gamma^k_{lm} y^l_{(1)} y^m_{(1)}\right), \\ &\vdots \\ \left(\frac{D^{N-1}v}{dt^{N-1}}(0)\right)^i &= y^i_{(N)} + \Gamma^i_{jk} y^j_{(1)} \left(\frac{D^{N-2}v}{dt^{N-2}}(0)\right)^k. \end{aligned} \tag{A.2.9}$$

The Jacobian matrix of the coordinate transformation

$$\left(x^i, y^i_{(1)}, y^i_{(2)}, \cdots, y^i_{(N)}\right) \mapsto \left(x^i, v(0)^i, \left(\frac{Dv}{dt}(0)\right)^i, \left(\frac{D^2v}{dt^2}(0)\right)^i, \cdots, \left(\frac{D^{N-1}v}{dt^{N-1}}(0)\right)^i\right) \tag{A.2.10}$$

is upper triangular, with blocks of the identity matrix δ^i_j 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 (A.2.2), can be reinterpreted invariantly using this isomorphism. In more detail:

1. Perform the coordinate transformation (A.2.10) 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 (A.2.10) has determinant 1, we can transform the distribution function $\psi(x, y)$ like a scalar function.

3. Compute all moments of $\psi(x, v(0), Dv/dt(0), \ldots, D^{N-1}v/dt^{N-1}(0))$ 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^i_{jk} vanish identically in Cartesian coordinates, so explicit coordinate expressions remain unmodified in this case. The above procedure gives an invariant interpretation of the

moments of ψ. This can be 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, and their images under the isomorphism $T^{(N)}M \simeq (T \oplus \cdots \oplus T)M$ do not coincide in general.

A.3 Riemannian metrics on the total space of a vector bundle

Let (M, g) be a Riemannian manifold, and let $\pi : E \to M$ be a vector bundle with a *Riemannian structure* h, which is a smoothly varying, symmetric positive definite bilinear form $h_x : E_x \times E_x \to \mathbb{R}$ 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 $\sigma : M \to E$ 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 $\nabla : \mathrm{Vect}(M) \times \Gamma(E) \to \Gamma(E)$, 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:

$$\nabla_{(fX+gY)}\sigma = f\nabla_X\sigma + g\nabla_Y\sigma, \tag{A.3.1a}$$

$$\nabla_X\left(a\sigma + \tau b\right) = a\nabla_X\sigma + b\nabla_X\tau, \tag{A.3.1b}$$

$$\nabla_X\left(f\sigma\right) = (X \cdot f)\sigma + f\nabla_X\sigma, \tag{A.3.1c}$$

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 (A.3.1a) 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 (A.3.1b) implies that the connection is $\mathbb{R}$-linear in its second argument. Condition (A.3.1c) can be interpreted as a form of the *Leibniz rule* – in terms of section-valued 1-forms, it is equivalent to

$$\nabla (f\sigma) = df \cdot \sigma + f\nabla\sigma, \tag{A.3.2}$$

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* $\sigma : U \to E|_U = \pi^{-1}(U)$, 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 $s_\alpha : U \to E|_U = \pi^{-1}(U), \alpha = 1, \dots q$ 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

$$(x, \xi) = (x^i, \xi^\alpha s_\alpha). \tag{A.3.3}$$

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

$$\nabla s_\alpha = \omega_\alpha^\beta s_\beta = \omega_{i\alpha}^\beta(x) dx^i s_\beta, \tag{A.3.4}$$

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:

$$\nabla \frac{\partial}{\partial x^\alpha} = \Gamma_{i\alpha}^\beta dx^i \frac{\partial}{\partial x^\beta}. \tag{A.3.5}$$

A local section $\sigma = \sigma(x)$ can be written as $\sigma = \xi^\alpha(x) s_\alpha$ for q local functions $\xi^1, \cdots, \xi^q$. Using the properties (A.3.1a-c), we can write the covariant derivative of $\sigma = \xi^\alpha(x) s_\alpha$ as

$$\nabla (\xi^\alpha s_\alpha) = \left(d\xi^\beta + \xi^\alpha \omega_\alpha^\beta\right) s_\beta. \tag{A.3.6}$$

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 $E|_U = \pi^{-1}(U)$:

$$\delta\xi^\beta = d\xi^\beta + \xi^\alpha \omega_{i\alpha}^\beta(x) dx^i. \tag{A.3.7}$$

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 $s_\alpha(x) \to s'_\alpha(x) = A_\alpha^\beta(x) s_\beta(x)$, 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 $\pi : E \to M$, there is a canonically defined *vertical subspace* $VE_{(x,\xi)}$ of the tangent space $T_{(x,\xi)}E$, defined as

$$VE_{(x,\xi)} = \ker\left(\pi_* : T_{(x,\xi)}E \to T_x M\right) = \ker\left(dx^i\right). \tag{A.3.8}$$

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 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:

$$HE_{(x,\xi)} = \ker\left(\delta\xi^\beta\right) = \ker\left(d\xi^\beta + \xi^\alpha \omega_{i\alpha}^\beta(x) dx^i\right). \tag{A.3.9}$$

Equivalently, $HE_{(x,\xi)}$ is the span of the tangent vectors to curves based at (x, ξ) that arose from horizontal lifting. Since the 1-forms (A.3.7) 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:

$$G_{(x,\xi)}(X, Y) = g_x(\pi_* X_h, \pi_* Y_h) + h_x(X_v, Y_v), \quad \text{for } X, Y \in T_{(x,\xi)}E. \tag{A.3.10}$$

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

$$G = g_{ij}dx^i dx^j + h_{\alpha\beta}\delta\xi^\alpha \delta\xi^\beta. \tag{A.3.11}$$

When $E = TM$ and the connection is the Levi-Civita connection on M, the metric G is precisely the *Sasaki metric* [192]. 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 Levi-Civita connection on TM (see appendix **A.2**). 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.

Appendix B

Supplementary material for section 3.6.4

This appendix details the calculation for the stress tensor $\boldsymbol{\sigma}$ in a steady state shear flow $\mathbf{u} = u(x_2)\hat{\mathbf{e}}_1$ in section **3.6.4**. In order to obtain an explicit expression for the stress tensor (3.6.11), we solve the equations (3.6.12a-e) for the internal state variables $\tilde{\mathbf{C}}$, $\tilde{\mathbf{B}}$, $\tilde{\mathbf{A}}$, $\tilde{\mathbf{b}}$ and $\tilde{\chi}$ in steady state, or equivalently at zero Strouhal number $\mathrm{St} = 0$.

In steady state, the equations for the internal state variables (3.6.12a-e) are *linear algebraic equations*, where the dependence on the steady state shear velocity $\tilde{u}(\tilde{x}_2)$ and its derivatives is parametric. These equations are

$$-\mathrm{De}\left(\tilde{u}'\mathbf{Q}\cdot\tilde{\mathbf{C}} + \tilde{u}'\tilde{\mathbf{C}}\cdot\mathbf{Q}^T\right) = -\tilde{\mathbf{C}} + \mathbf{I}, \tag{B.0.1a}$$

$$-\mathrm{De}\left(\tilde{u}'\mathbf{Q}\cdot\tilde{\mathbf{B}} + \tilde{u}'\tilde{\mathbf{B}}\cdot\mathbf{Q}^T + \lambda^2\tilde{u}''\left(\mathbf{Q}\cdot\tilde{\mathbf{A}} + \left(\mathbf{Q}\cdot\tilde{\mathbf{A}}\right)^T\right)\right) = -\frac{1}{s}\tilde{\mathbf{B}} + \mathbf{I}, \tag{B.0.1b}$$

$$-\mathrm{De}\left(\tilde{u}'\mathbf{Q}\cdot\tilde{\mathbf{A}} + \tilde{u}'\tilde{\mathbf{A}}\cdot\mathbf{Q}^T + u''\begin{pmatrix}\tilde{\chi}_{2212}\\ \tilde{\chi}_{2222}\\ \tilde{\chi}_{2232}\end{pmatrix}\otimes\hat{\mathbf{e}}_1\right) = -\frac{2s+1}{2s}\tilde{\mathbf{A}} + \hat{\mathbf{e}}_2\otimes\tilde{\mathbf{b}}, \tag{B.0.1c}$$

$$-\mathrm{De}\left(\tilde{u}'\mathbf{Q}\cdot\tilde{\mathbf{b}} + \tilde{u}''\hat{\mathbf{e}}_1\tilde{C}_{22}\right) = -\frac{1}{2s}\tilde{\mathbf{b}}, \tag{B.0.1d}$$

$$-\mathrm{De}\tilde{u}'\begin{pmatrix}\tilde{\chi}_{2222}\\ 0\\ 0\end{pmatrix} = -2\begin{pmatrix}\tilde{\chi}_{2212}\\ \tilde{\chi}_{2222}\\ \tilde{\chi}_{2232}\end{pmatrix} + \begin{pmatrix}3\tilde{C}_{12}\\ 6\tilde{C}_{22}\\ 3\tilde{C}_{23}\end{pmatrix}. \tag{B.0.1e}$$

The system of linear equations (B.0.1a-e) has a unique solution. We prove this by using a general fact in linear algebra: Let V be a (real or complex) vector space. Denote the identity map on V by I, and let $N : V \to V$ be a *nilpotent* linear map i.e. $N^k = 0$ for some positive integer k. Consider the following inhomogeneous linear equation

$$(\alpha I + \beta N)\, v = w, \tag{B.0.2}$$

where v, w are vectors in V, α, β are constants, and $\alpha \neq 0$. Given w, this equation always has a unique solution for v. To show this, take $\alpha = \beta = 1$ without loss of generality and use the identity

$$(I + N)^{-1} = I - N + N^2 - \ldots, \tag{B.0.3}$$

where the Neumann series on the right hand side is *finite*, because $N^k = 0$ for some positive integer k. This means $I + N$ is invertible and thus an equation of the form $(I + N)v = w$ has a unique solution for v given w.

The general fact indicated above can be applied to solving (B.0.1a-e). On the vector space of 3×3 matrices, the linear map $\mathbf{M} \mapsto \mathbf{Q} \cdot \mathbf{M} + \mathbf{M} \cdot \mathbf{Q}^T$, where $\mathbf{Q} = \hat{\mathbf{e}}_1 \otimes \hat{\mathbf{e}}_2$ as before, is nilpotent. The equations (B.0.1a, B.0.1b, B.0.1c) can then be put into the form (B.0.2), and we can apply (B.0.3) to solve for the explicit forms of $\tilde{\mathbf{C}}$, $\tilde{\mathbf{B}}$ and $\tilde{\mathbf{A}}$ provided that we know the explicit forms of the inhomogeneous terms. The explicit algorithm is:

1. Solve (B.0.1a) for $\tilde{\mathbf{C}}$. Equation (B.0.1a) can be rearranged into the form (B.0.2) with known right-hand side.

2. Solve (B.0.1d, B.0.1e) for $\tilde{\mathbf{b}}$ and $\tilde{\chi}$, given the solution for $\tilde{\mathbf{C}}$ from step 1.

3. Solve (B.0.1c) for $\tilde{\mathbf{A}}$. Equation (B.0.1c) can be rearranged into the form (B.0.2) with right-hand side depending on $\tilde{\mathbf{b}}$ and $\tilde{\chi}$, which we know from step 2.

4. Solve (B.0.1b) for $\tilde{\mathbf{B}}$. Equation (B.0.1b) can be rearranged into the form (B.0.2) with right-hand side depending on $\tilde{\mathbf{A}}$, which we know from step 3.

The explicit solution to (B.0.1a-e) found from this algorithm is

$$\tilde{\mathbf{C}} = \begin{pmatrix} 1 + 2\mathrm{De}^2(\tilde{u}')^2 & \mathrm{De}\tilde{u}' & 0 \\ \mathrm{De}\tilde{u}' & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$\begin{pmatrix} \tilde{\chi}_{2212} \\ \tilde{\chi}_{2222} \\ \tilde{\chi}_{2232} \end{pmatrix} = \begin{pmatrix} 3\mathrm{De}\tilde{u}' \\ 3 \\ 0 \end{pmatrix},$$

$$\tilde{\mathbf{b}} = \begin{pmatrix} 2s\mathrm{De}\tilde{u}'' \\ 0 \\ 0 \end{pmatrix},$$

$$\tilde{\mathbf{A}} = \begin{pmatrix} \frac{2s(4s^2+12s+3)}{(2s+1)^2}\mathrm{De}^2\tilde{u}'\tilde{u}'' & 0 & 0 \\ \frac{2s(3+2s)}{2s+1}\mathrm{De}\tilde{u}'' & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$\tilde{\mathbf{B}} = s \begin{pmatrix} 1 + 2s^2\mathrm{De}^2(\tilde{u}')^2 + \frac{4s(3+2s)}{2s+1}\lambda^2\mathrm{De}^2(\tilde{u}'')^2 & s\mathrm{De}\tilde{u}' & 0 \\ s\mathrm{De}\tilde{u}' & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Substituting these expressions into the stress tensor (3.6.11) gives the following explicit expressions for the steady state stress of the Hookean 3-bead chain under a steady shear flow:

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & 0 \\ \sigma_{21} & \sigma_{22} & 0 \\ 0 & 0 & \sigma_{33} \end{pmatrix}, \tag{B.0.4}$$

with the nonzero components given below:

$$\begin{aligned} \frac{\sigma_{11}}{nk_BT} =& -1 + 2(1+s^2)\mathrm{De}^2(\tilde{u}')^2 + \frac{4s(3+2s)}{2s+1}\lambda^2\mathrm{De}^2(\tilde{u}'')^2 \\ & - \frac{2(4s^2+12s+3)}{(2s+1)^2}\lambda^2\mathrm{De}^2(\tilde{u}''\tilde{u}'' + \tilde{u}'\tilde{u}'''), \end{aligned} \tag{B.0.5a}$$

$$\frac{\sigma_{12}}{nk_BT} = (1+s)\mathrm{De}\tilde{u}', \tag{B.0.5b}$$

$$\frac{\sigma_{21}}{nk_BT} = (1+s)\mathrm{De}\tilde{u}' - \frac{2(3+2s)}{2s+1}\lambda^2\mathrm{De}\tilde{u}''', \tag{B.0.5c}$$

$$\frac{\sigma_{22}}{nk_BT} = -1, \tag{B.0.5d}$$

$$\frac{\sigma_{33}}{nk_BT} = -1. \tag{B.0.5e}$$

Appendix C

Supplementary material for section 4.4.2

This appendix contains supplementary material for section **4.4.2**. We set our conventions for the Laguerre polynomials and tabulate the explicit expressions for $\bar{\eta}_a, M(\eta_1)_{ab}$ (4.4.42, 4.4.44) and $\tilde{\beta}_a$ (4.4.41, 4.4.45) up to order 4.

Laguerre polynomials

For $\alpha > -1$ and $a = 0, 1, \ldots$, the *(generalised) Laguerre polynomials* $L_b^\alpha(\chi)$ are defined as (see ch. 6.2 of [5])

$$L_b^\alpha(\chi) := \frac{\chi^{-\alpha}\mathrm{e}^{\chi}}{\Gamma(b+1)}\left(\frac{d}{d\chi}\right)^b\left(\mathrm{e}^{-\chi}\chi^{b+\alpha}\right). \tag{C.0.1}$$

Each $L_b^\alpha(\chi)$ is a polynomial of degree b. The first few Laguerre polynomials are

$$\begin{aligned} L_0^\alpha(\chi) &= 1, \\ L_1^\alpha(\chi) &= -\chi + (\alpha+1), \\ L_2^\alpha(\chi) &= \frac{\chi^2}{2} - (\alpha+2)\chi + \frac{(\alpha+1)(\alpha+2)}{2}. \end{aligned}$$

The Laguerre polynomials satisfy the orthogonality relation

$$\int_0^\infty d\chi\ \chi^\alpha \mathrm{e}^{-\chi} L_a^\alpha(\chi) L_b^\alpha(\chi) = \frac{\Gamma(a+\alpha+1)}{\Gamma(a+1)}\delta_{ab} \tag{C.0.2}$$

and form a complete orthogonal basis for the Hilbert space $L^2(\mathbb{R}_+, \chi^\alpha \mathrm{e}^{-\chi} d\chi)$.

Explicit expressions for $\bar{\eta}_a, M(\eta_1)_{ab}$ and $\tilde{\beta}_a$ up to order 4

The first few $\bar{\eta}_a, M(\eta_1)_{ab}$ in (4.4.42, 4.4.44) are

$$\begin{pmatrix} \bar{\eta}_2 \\ \bar{\eta}_3 \\ \bar{\eta}_4 \end{pmatrix} = \begin{pmatrix} \eta_1^2 + \frac{1}{2}n \\ \eta_1^3 + \frac{3}{2}n\eta_1 - n \\ \eta_1^4 + 3n\eta_1^2 - 4n\eta_1 + \frac{3}{4}n^2 + 3n \end{pmatrix}, \tag{C.0.3}$$

$$M(\eta_1) = \begin{pmatrix} M_{22} & 0 & 0 & \dots \\ M_{32} & M_{33} & 0 & \dots \\ M_{42} & M_{43} & M_{44} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \tag{C.0.4}$$

where

$$\begin{aligned} M_{22} &= \frac{1}{4} n(n+2), \\ M_{32} &= \frac{3}{4} n(n+2)(\eta_1 - 1), \\ M_{33} &= \frac{1}{8} n(n^2 + 6n + 8), \\ M_{42} &= \frac{3}{4} n(n+2)(2\eta_1^2 - 4\eta_1 + n + 4), \\ M_{43} &= \frac{1}{2} n(n^2 + 6n + 8)(\eta_1 - 2), \\ M_{44} &= \frac{1}{16} n(n^3 + 12n^2 + 44n + 48). \end{aligned}$$

The first few $\tilde{\beta}_a$ in (4.4.41, 4.4.45) are

$$\tilde{\beta}_2 = \frac{2\eta_2 - 2\eta_1^2 - n}{n(n+2)/2}, \tag{C.0.5a}$$

$$\tilde{\beta}_3 = \frac{4\eta_1^3 - 6\eta_1^2 - 6\eta_2\eta_1 + 6\eta_2 + 2\eta_3 - n}{n(n^2 + 6n + 8)/4}, \tag{C.0.5b}$$

$$\begin{aligned} \tilde{\beta}_4 = \Big(& 48\eta_2 + 32\eta_3 + 4\eta_4 - 4n - 96\eta_1\eta_2 - 16\eta_1\eta_3 \\ & - 12n\eta_2 + 24\eta_1^2\eta_2 + 12n\eta_1^2 - 48\eta_1^2 + 64\eta_1^3 - 12\eta_1^4 + 3n^2 \Big) \\ & \div \left(\frac{n(n^3 + 12n^2 + 44n + 48)}{4} \right). \end{aligned} \tag{C.0.5c}$$

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