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Kinetic models of oriented self-assembly

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Abstract

New kinetic models of dissipation are proposed for the dynamics of an ensemble of interacting oriented particles, for example, moving magnetized nano-particles. This is achieved by introducing double-bracket dissipation into kinetic equations by using an oriented Poisson bracket and employing the moment method to derive continuum equations for the evolution of magnetization and mass density. These continuum equations generalize the Debye–Hückel equations for attracting round particles, and Landau–Lifshitz–Gilbert equations for spin waves in magnetized media. The dynamics of self-assembly is investigated as the emergent concentration into singular clumps of aligned particles (*orientons*) starting from random initial conditions. Finally, the theory is extended to describe the dissipative motion of self-interacting curved filaments.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Many physical systems such as plasmas, particle-laden fluids and self-assembling molecules may be understood in terms of collective dynamics of a large number of particles moving in an ambient medium. Dissipation plays the crucial role for these systems of making them tend towards an eventual equilibrium state in the absence of external forces. The dissipation in *heterogeneous* systems is fundamentally different from internal dissipation in homogeneous fluids, which is usually described by diffusion of mass and momentum by microscopic scattering processes. The goal of this paper is to demonstrate a unifying principle for deriving dissipation in systems consisting of particles migrating through an ambient fluid

or matrix. The only role the matrix plays is to resist the motion of individual particles at the microscopic level. That is, the matrix itself is assumed to have no dynamics of its own. This resistance is applied both in configuration space and in momentum space when considering kinetic processes.

Thus, we have in mind the physical situation of microscopic particles that are magnetized (or otherwise oriented) moving under the influence of external forces and mutual attraction in a passive ambient continuum. Such systems have attracted much attention recently because of their potential technological significance. For example, magnetic nano-particles in this setting have yielded crystalline structures whose concentrated densities far exceed that achievable using lithographic procedures [1, 41, 46].

Much of the modern modeling of dissipation in systems of moving nano-particles is based on the work of George Gabriel Stokes, who formulated his famous drag law for the resistance of spherical particles moving in a viscous fluid at low Reynolds numbers. Reynolds number is defined as the ratio $R = UL/\nu$ where U is the typical velocity, L is the typical size and ν is the kinematic viscosity. Reynolds number is physically the ratio between a typical inertial term and viscous force, and $R \ll 1$ means the total dominance of viscous forces. It is commonly assumed that all processes in fluids at micro- and nano-scales are dominated by viscous forces and the Stokes approximation applies. The Stokes result states that a round particle moving through an ambient fluid will experience a resistance force that is proportional to the velocity of the particle [2]. Conversely, in the absence of inertia, the velocity of a particle will be proportional to the force applied to it since resistance force and applied force must balance. This law—that 'force is proportional to velocity'—is sometimes called *Darcy's law*[5].

In generalizing this concept to apply to an assembly of a large number of particles, we define the relative density of particles as the number of particles per unit volume, ρ. Given the energy of particles in given configuration $E[\rho]$, the local velocity of particles under the force $\mathbf{F} = -\nabla\delta E/\delta\rho$ is $\mathbf{u} = -\mu\mathbf{F}$. The coefficient of proportionality is called the *mobility* μ.

In most cases, the mobility is allowed to depend on the density ρ. In particular, here we allow for μ to be an average value of the pointwise dynamical variable ρ. This average value is given by a convolution $\mu = K * \rho$ with some positive-definite, symmetric kernel K. The equation of motion for the pointwise density ρ is then given by the following conservation law whose setting in statistical physics can be traced back to Debye and Hückel [8]:

$$\frac{\partial\rho}{\partial t} = -\operatorname{div}\rho\mathbf{u} = \operatorname{div}\left(\rho\mu\nabla\frac{\delta E}{\delta\rho}\right). \tag{1}$$

This equation neglects the diffusion of ρ that may occur if the particles also experience Brownian motion. Note that the rate of change of the energy $E[\rho]$ and any arbitrary functional of density $F[\rho]$ is given by

$$\frac{\mathrm{d}E}{\mathrm{d}t} = -\int \rho\mu[\rho]\left|\nabla\frac{\delta E}{\delta\rho}\right|^2 \mathrm{d}\mathbf{x}, \qquad \frac{\mathrm{d}F}{\mathrm{d}t} = -\int \rho\mu[\rho]\nabla\frac{\delta E}{\delta\rho}\cdot\nabla\frac{\delta F}{\delta\rho}\,\mathrm{d}\mathbf{x}, \tag{2}$$

which can be seen by direct application of equation (1). See also [21, 22, 38] for relevant discussions.

It is interesting that the work of Gilbert on dissipation in the Landau–Lifshitz equation for spin waves may be recast into the Darcy law form. Indeed, Gilbert [15] assumed a *dissipative*

[5] H P G Darcy is best known for his empirical law on fluid flow through porous media, published as an appendix to his book *Les Fontaines publiques de la ville de Dijon*. Darcy had built a water supply system for Dijon in 1840, and in 1856, shortly before his death, he wrote a book to guide other engineers in constructing similar projects. Darcy's book was recently translated into English by P Bobeck [2003] *Henry Darcy and the Public Fountains of the City of Dijon*, Geotechnical Translations, Austin, Texas.

resistive force $F[\mathbf{M}]$ for a set of spins $\mathbf{M}$ that is proportional to the rate of change of $\mathbf{M}$ in time, which we shall denote as $\dot{\mathbf{M}}$,

$$F_i[\mathbf{M}] = \eta_{ij}\dot{M}_j. \tag{3}$$

Gilbert proposed that in the absence of any information about the matrix η_{ij} it is prudent to assume that it is isotropic, so that $\eta_{ij} = \eta\delta_{ij}$. This simplifying assumption ultimately leads to the Landau–Lifshitz–Gilbert dissipation term [15, 33] which we write as

$$\frac{\mathrm{d}\mathbf{M}}{\mathrm{d}t} = \gamma\mathbf{M}\times\mathbf{H} + \frac{\lambda}{M^2}\mathbf{M}\times\mathbf{M}\times\mathbf{H}, \tag{4}$$

where $\mathbf{H}$ is the magnetic field, which can be expressed in terms of the external field $\mathbf{H}_{\text{ext}}$ and the energy of particle interactions $E[\mathbf{M}]$ as $\mathbf{H} = \mathbf{H}_{\text{ext}} + \delta E/\delta\mathbf{M}$. Here $\delta E/\delta\mathbf{M}$ is the variational, or Fréchet derivative and γ, λ are constants. In this theory, the *mobility function* η satisfies Gilbert's relation $\eta\gamma^2M^2 = \lambda$ [15].

Gilbert's theory is not universal and alternative phenomenological theories of dissipation of magnetization exist that are not in generalized Darcy form [5, 7]. The Hamiltonian part of Gilbert's equation is the first term on the right-hand side of (4). This term mimics the dynamics of the rigid body in terms of angular momentum. The important feature of Gilbert's model is that it conserves the magnitude of the magnetization vector $|\mathbf{M}|$, while it dissipates the total energy $\gamma\int\mathbf{M}\cdot\mathbf{H}\,\mathrm{d}^3\boldsymbol{x}$.

If we only take into account the dissipative (right-hand side) terms in Gilbert's equation (4), then the rate of change in an arbitrary functional of the magnetization $\mathbf{M}$ is given by

$$\frac{\mathrm{d}F}{\mathrm{d}t} = -\int\left(\mathbf{M}\times\frac{\delta E}{\delta\mathbf{M}}\right)\cdot\left(\mathbf{M}\times\frac{\delta F}{\delta\mathbf{M}}\right)\mathrm{d}\mathbf{x}. \tag{5}$$

Hence, the rate of change of the magnetization energy is given by

$$\frac{\mathrm{d}E}{\mathrm{d}t} = -\int\left(\mathbf{M}\times\frac{\delta E}{\delta\mathbf{M}}\right)^2\mathrm{d}\mathbf{x}. \tag{6}$$

Thus, in essence, both the Stokes drag law and Gilbert dissipation are based on a single mathematical assumption. Namely, a *dissipative force* acting on a physical quantity is proportional to the rate of change of that physical quantity. The Stokes drag law is valid for mobile particles that interact via collisions. Gilbert's work is developed for particles with an immobile center of mass that can orient themselves and change their magnetic properties. As far as we are aware, the work since Gilbert and Landau–Lifshitz on magnetic dissipation has remained largely phenomenological. A theory of magnetic dissipation for freely moving particles that is applicable to the self-assembly of nano-particles still remains to be derived. The challenge now is to place the phenomenological arguments that have been shown historically to be practical for magnetic dissipation into a systematic theoretical framework.

This paper derives equations for the dynamics of magnetized particles moving through a passive ambient fluid. Our derivation of these dynamical equations is not based on phenomenological arguments. Equations (2) and (6) possess intriguing physical and mathematical similarities, but a direct generalization to moving particles with orientation does not seem feasible. Instead, we proceed by introducing dissipation into the kinetic (Vlasov) equation describing the motion of probability density $f(p,q,t)$ in the single-particle momentum p and coordinate q space. Only that approach can be physically justified. Our starting point is the formulation of the dissipative kinetic theory of gases consisting of arbitrarily shaped microscopic rigid bodies by accurately taking into account the linear and angular momentum of a microscopic particle. The continuum equations of motion for the

density and magnetization are then obtained by integrating out the momentum coordinate and truncating the expansion to the first order (a procedure known as *moment truncation* in plasma physics). Our general framework is of considerable physical interest because it recovers both the continuum conservation law (1) for particles without orientation, and the Gilbert dissipation (4) for oriented particles with an immobile center of mass. Moreover, in example systems, we observe the formation of domains of coherent orientation and we analytically predict the evolution of each domain.

We note that an alternative form of dissipation in continuum media, caused by the Brownian motion and expressed as diffusion terms in the Fokker–Planck equations is not suitable for our purposes, as applied to density, orientation or Vlasov probability density in phase space. The Fokker–Planck equation is a drift-diffusion extension of the Vlasov equation for kinetic dynamics that is widely used as a powerful tool in understanding the physics of certain dissipative phenomena, especially in plasma physics. In this regard we mention important results by Chavanis *et al* (see [6] and references therein), where a particular form of equation (1) with $\mu = \text{const.}$ has been obtained from a generalized Fokker–Plank treatment in the simpler case of isotropic interactions. However, informed by recent results achieving highly concentrated states in nano-scale self-assembly [1, 41, 46], we assume that Brownian particle diffusion may be neglected for our purposes. For other experiments with stronger diffusive effects, one would seek an alternative theory.

2. A dissipative kinetic equation for collisionless systems

Recently, it was demonstrated [26] that Darcy's conservation law (1) can be obtained from the introduction of dissipation in the kinetic Vlasov equations, describing the evolution of the density $f(p, q, t)$ in the phase space of the form

$$\frac{\partial f}{\partial t} + \underbrace{\left\{ f, \frac{\delta H}{\delta f} \right\}}_{\text{Inertial part}} = \underbrace{\left\{ f, \left\{ \mu[f], \frac{\delta E}{\delta f} \right\} \right\}}_{\text{Dissipative part}}, \tag{7}$$

where $H[f]$ is the Vlasov Hamiltonian and $\delta H/\delta f$ is its variational (Fréchet) derivative, governing the single-particle motion. The *mobility* (in phase space) $\mu[f]$ is a modeling choice and the energy functional $E[f]$ is usually taken to be the potential part of the Hamiltonian H, describing just the self-interactions between the particles in the momentum space. The variational derivative $\delta E/\delta f$ is called the *chemical potential*. If the inertial part is neglected, then by integrating this equation with respect to the momentum (p) we obtain precisely equation (1), with $\rho(q, t) = \int f(p, q, t)\,\mathrm{d}p$ and $\mu[\rho] = \int \mu[f(p, q, t)]\mathrm{d}p$. A particular form of equation (7) with $\mu[f] = f$ was first suggested by Kandrup [29] in the context of galactic dynamics, and then analyzed further by Bloch *et al* [3, 4].

Properties of equation (7). We list a series of relevant results for equation (7) that were proved in [26].

Lemma 2.1. *Equation (7) preserves the single-particle solutions*

$$f = \sum_k w_k(t)\delta(p - p_k(t))\delta(q - q_k(t)),$$

(with $\dot{w}_k = 0$) that are not allowed in other approaches in kinetic dissipation.

Lemma 2.2. *Equation (7) preserves entropy $S = \int f \log f \,\mathrm{d}p\,\mathrm{d}q$ and has infinitely many Casimirs: for an arbitrary function $\phi(f)$, the integral $\int \phi(f)\,\mathrm{d}p\,\mathrm{d}q$ is constant, independently of the choice of interaction energy.*

Remark 2.3. Considering the advective nature of equation (7), the results in the lemmas above should not be surprising. Indeed, since the Vlasov density f is advected by the phase-space fluid, any integral of $\phi(f)$ is constant and so is the entropy. The invariance of the single-particle solution is also a consequence of the advective form of equation (7).

Lemma 2.4. *If the inertial part is discarded, then truncating the moment equations and keeping only the terms dependent on* $\rho = \int f(p,q,t)\,\mathrm{d}p$ *(zeroth moment terms) yields exactly Debye–Hückel equation (1).*

Let us now demonstrate how the dissipation given by (7) is connected to the Darcy's law. We neglect the inertial part of (1) and consider the rate of change for the energy $E[f]$ and an arbitrary functional $F[f]$ using Kandrup's choice for the mobility $\mu[f] = f$:

$$\frac{\mathrm{d}E}{\mathrm{d}t} = -\int \left\{ f, \frac{\delta E}{\delta f} \right\}^2 \mathrm{d}\mathbf{x}, \qquad \frac{\mathrm{d}F}{\mathrm{d}t} = -\int \left\{ f, \frac{\delta E}{\delta f} \right\} \left\{ f, \frac{\delta F}{\delta f} \right\} \mathrm{d}\mathbf{x}. \tag{8}$$

This result can also be easily generalized to mobility functionals having the form $\mu[f] = fM[f]$, with $M[f] \geqslant 0$ being a scalar functional of f [26]. For general mobility functionals $\mu[f]$, the quadratic form given by energy dissipation functional (8) is not necessarily positive definite.

Thus, just as equation (1), the dissipation in (7) enforces the rate of change of an arbitrary functional of the solution to be linear in both $\delta E/\delta f$ and $\delta F/\delta f$. In particular, energy dissipation is given by a quadratic form of $\delta E/\delta f$. This formulation in terms of energy dissipation is actually equivalent to saying 'force is proportional to velocity', but it has much more physical and mathematical power, which we are going to exploit in this paper.

The mathematical equivalence of the dissipation laws (2), (6) and (8) is now clear.

Assumption 2.5. *The energy dissipation of an arbitrary functional* $F[f]$ *is a quadratic form in the variational derivative of* $F[f]$ *and the energy* $E[f]$ *(see (9) below).*

There seems to be no direct path to consistently generalize the evolution equation for moving magnets to include both density and orientation, somehow combining (1) and (4). The path we follow is to extend the kinetic equation (7) to account for orientation interaction and then compute the evolution equations using the moments approach.

3. History and mathematical background

3.1. Selective decay hypothesis

This work was inspired by the dissipative bracket structure introduced in Bloch *et al* [4], which in turn was motivated in part by the double bracket introduced by Vallis, Carnevale and Young [44] for incompressible fluid flows. The dominant idea for [44] was the selective decay hypothesis, which arose in turbulence research [34] and is consistent with the preservation of coadjoint orbits. According to the selective decay hypothesis, energy in strongly nonequilibrium statistical systems tends to decay much faster than certain other ideally conserved properties. In particular, energy decays much faster in such systems than those 'kinematic' or 'geometric' properties that would have been preserved in the ideal nondissipative limit *independently of the choice of the Hamiltonian*. Examples are Casimir functions for the Lie–Poisson formulations of various ideal fluid models [20].

The selective decay hypothesis, in turn, was inspired by a famous example in two-dimensional turbulence theory. Namely, that enstrophy decays much more slowly than kinetic energy in 2D incompressible fluid turbulence. Kraichnan [31] showed that the decay of kinetic

energy under the preservation of enstrophy causes dramatic effects in 2D turbulence. Namely, it causes the well-known 'inverse cascade' of kinetic energy to *larger* scales, rather than the 'forward cascade' of energy to smaller scales that is observed in 3D turbulence. In 2D ideal incompressible fluid flow the enstrophy (the L^2 norm of the vorticity) is preserved on coadjoint orbits. That is, enstrophy is a Casimir of the Lie–Poisson bracket in the Hamiltonian formulation of the 2D Euler fluid equations. Vallis *et al* [44] chose a form of dissipation that was expressible as a double Lie–Poisson bracket. This choice of dissipation preserved the enstrophy and thereby enforced the selective decay hypothesis for all 2D incompressible fluid solutions, laminar as well as turbulent.

Once its dramatic effects were recognized in 2D turbulence, selective decay was posited as a governing mechanism in other systems, particularly in statistical behavior of fluid systems with high variability. For example, the slow decay of magnetic helicity was popularly invoked as a possible means of obtaining magnetically confined plasmas [42]. Likewise, in geophysical fluid flows, the slow decay of potential vorticity (PV) relative to kinetic energy strongly influences the dynamics of weather and climate patterns much as in the inverse cascade tendency in 2D turbulence. The use of selective decay ideas for PV thinking in meteorology and atmospheric science has become standard practice since the fundamental work in [27, 45].

Thus, in geophysical situations, one would like a dissipative mechanism that separates the different time scales of decay of the energy and the PV. At leading order, one would like a dissipative mechanism for which the energy decays but the PV persists. This is exactly the sort of dissipative mechanism that was introduced in Vallis *et al* [44] and is being developed more generally here. Likewise, in plasma physics and stellar dynamics, one would like to have a dissipative mechanism that preserves the fundamental conservation of particle number, yet has energy decay. Again, the general mechanism introduced here satisfies these properties. (See Kandrup [28, 29], as well as Bloch *et al* [4] and references therein.) We will discuss all of these examples and many others in the body of this paper.

3.2. Mathematical framework for geometric dissipation

As explained in [38], dissipation of energy E may naturally summon an appropriate metric tensor. In previous work, Holm and Putkaradze [23, 25] showed that for any two functionals $F[\kappa]$, $G[\kappa]$ of a geometric quantity κ a distance between them may be defined via the Riemannian metric,

$$g_\kappa(F,E) = \left\langle \left(\mu[\kappa]\diamond\frac{\delta F}{\delta f}\right), \left(\kappa\diamond\frac{\delta E}{\delta f}\right)^\sharp \right\rangle_{\mathfrak{X}^*\times\mathfrak{X}}. \tag{9}$$

Here $\langle\cdot,\cdot\rangle$ denotes the L^2 pairing of vector fields ($\mathfrak{X}$) with their dual one-form densities ($\mathfrak{X}^*$), sharp $(\cdot)^\sharp$ raises the vector index from covariant to contravariant and $\mu[\kappa]$ is the *mobility functional*. The mobility $\mu[\kappa]$ is assumed to satisfy the requirements for (9) to be positive definite and symmetric, as discussed in [25]. The diamond operation ($\diamond$) in equation (9) is the dual of the Lie algebra action, defined as follows. Let a vector field ξ act on a vector space V by Lie derivation, so that the Lie algebra action of ξ on any element $\kappa\in V$ is given by the Lie derivative,

$$\xi\cdot\kappa = \pounds_\xi\kappa.$$

The operation dual to the Lie derivative is denoted by $\diamond$ and defined in terms of the L^2 pairings between $\mathfrak{X}$ and $\mathfrak{X}^*$ and between V and V^* as

$$\langle\zeta\diamond\kappa,\xi\rangle_{\mathfrak{X}^*\times\mathfrak{X}} := \langle\zeta,-\pounds_\xi\kappa\rangle_{V^*\times V}. \tag{10}$$

Given the metric (9) and a dissipated energy functional $E[\kappa]$, the time evolution of *arbitrary* functional $F[\kappa]$ is given by [23, 25] as

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \{\{F, E\}\}[\kappa] := -g_\kappa(F, E) = -\left\langle \left(\mu[\kappa] \diamond \frac{\delta E}{\delta \kappa}\right), \left(\kappa \diamond \frac{\delta F}{\delta \kappa}\right)^\sharp \right\rangle_{\mathfrak{X}^* \times \mathfrak{X}}, \tag{11}$$

which specifies the dynamics of any functional $F[\kappa]$, given the energy dependence $E[\kappa]$. The bracket $\{\{F, E\}\}$ is shown to satisfy the Leibnitz product-rule property for a suitable class of mobility functionals $\mu[\kappa]$ in [23, 25]. Equation (11) and positivity of $g_\kappa(E, E)$ imply that the energy E decays in time until it eventually reaches a critical point, $\delta E/\delta \kappa = 0$.

Remark 3.1. For densities (dual to functions in the L^2 pairing), the Lie derivative is the divergence and its dual operation is (minus) the gradient. Thus, for densities the symbol diamond ($\diamond$) is replaced by gradient (∇) in the metric defined in equation (11).

Entropy-based dissipative brackets. Historically, variational approaches for introducing dissipation that decreases energy and increases entropy were used already at the end of the 19th century by Lord Rayleigh. However, interest in the use of symmetric brackets for introducing dissipation of this type into Hamiltonian systems seems to have arisen a century later almost simultaneously in the works of Kaufman [30], Morrison [35] and Grmela [16]. This later approach introduces dissipation using a symmetric bracket operation that increases an entropy, in concert with nonequilibrium thermodynamics approaches going back to Onsager and Casimir. See [17, 18] and [37] for references to this approach and its further engineering developments.

The dissipative bracket in equation (11) differs fundamentally from the symmetric brackets proposed earlier for entropy-based dissipation in [16, 30, 35]. In particular, the dissipative bracket in equation (11) preserves entropy, while the dissipative brackets in the earlier literature are based on increasing entropy. Moreover, the dynamics of dissipative brackets based on entropy decrease does not appear to be expressible as a geometric transport equation in Lie-derivative form. Thus, on geometric and thermodynamic grounds, the two approaches are essentially different. It remains an interesting open question as to whether these two different approaches could be used in some complementary fashion.

4. Kinetic equation for anisotropic particles and Landau–Lifshitz equations

We now turn to the problem of a system composed of immobile particles of arbitrary shape. The orientation $\boldsymbol{m}$ of particles now appears as an additional degree of freedom, but the particle momentum $\mathbf{p}$ is going to be neglected in this section since centers of mass for the particles are assumed to be immobile. In our approach we consider orientation as given by the angular momentum of each particle. Thus, instead of considering unit vectors for orientation, we consider angular momentum vectors and each particle is treated as a rigid body.

Let us consider the non-dissipative case first. The evolution equation for the distribution function $\varphi(\boldsymbol{x}, \boldsymbol{m}, t)$ in this approach is written in the conservation form in the $\mathbf{U} = (\mathbf{U}_x, \mathbf{U}_m)$ on the $(\boldsymbol{x}, \boldsymbol{m})$ space

$$\frac{\partial \varphi}{\partial t} = -\mathrm{div}_{(x,m)}(\varphi \mathbf{U}) = -\nabla_{\boldsymbol{x}} \cdot (\varphi \mathbf{U}_x) - \frac{\partial}{\partial \boldsymbol{m}} \cdot (\varphi \mathbf{U}_m).$$

As mentioned earlier, we set $\mathbf{U}_x = \mathbf{0}$ in this section, since the centers of mass for the particles are assumed to be stationary. Since the angular momentum for a rigid body evolves according

to the Hamiltonian motion $\dot{\boldsymbol{m}} = \boldsymbol{m} \times \nabla_m h = \mathbf{U}_m$, we can write our kinetic equation as

$$\frac{\partial \varphi}{\partial t} + \left[\varphi, \frac{\delta H}{\delta \varphi}\right] = 0,$$

where we have used the definition of the rigid-body bracket

$$[\varphi, h] := \boldsymbol{m} \cdot \nabla_m \varphi \times \nabla_m h, \tag{12}$$

and the global Hamiltonian is written as

$$H[\varphi] = \int\!\!\int \varphi(\boldsymbol{x}, \boldsymbol{m}) h(\boldsymbol{x}, \boldsymbol{m})\, \mathrm{d}^3\boldsymbol{x}\, \mathrm{d}^3\boldsymbol{m}.$$

Having obtained the conservative dynamics in the bracket form, we are motivated to insert the dissipation as the double-bracket form of (7) as follows:

$$\frac{\partial \varphi}{\partial t} + \underbrace{\left[\varphi, \frac{\delta H}{\delta \varphi}\right]}_{\text{Inertia}} = \underbrace{\left[\varphi, \left[\mu[\varphi], \frac{\delta E}{\delta \varphi}\right]\right]}_{\text{Dissipation}}. \tag{13}$$

In this context, it is reasonable to take the moments with respect to $\boldsymbol{m}$ and in particular we want the equation for the magnetization density, defined by

$$\mathbf{M}(\boldsymbol{x}, t) := \int \boldsymbol{m} \varphi\, \mathrm{d}^3\boldsymbol{m},$$

for the case that $H = E$. We now introduce the assumption that the single-particle energy h is linear in $\boldsymbol{m}$. It is easy to see that this assumption recovers, for example, the expression of the potential energy of a magnetic moment in a magnetic field.

Again, let us consider only the dissipation terms in (13), i.e., the term on the right-hand side and use Kandrup's assumption for the mobility $\mu[\varphi] = \varphi$. Then, we find an evolution of an arbitrary functional $F[\varphi]$ as well as dissipation of energy $E[\varphi]$ in the quadratic form analogous to (8):

$$\frac{\mathrm{d}F}{\mathrm{d}t} = -\int \left[\varphi, \frac{\delta E}{\delta \varphi}\right]\left[\varphi, \frac{\delta F}{\delta \varphi}\right] \mathrm{d}\mathbf{x}, \qquad \frac{\mathrm{d}E}{\mathrm{d}t} = -\int \left[\varphi, \frac{\delta E}{\delta \varphi}\right]^2 \mathrm{d}\mathbf{x}. \tag{14}$$

The extension to more general mobility functionals is also possible, but the quadratic form describing the dissipation will not be symmetric, in general, for an arbitrary choice of the mobility functional.

Now, by using the method of moments we compute the equation for the magnetization density $\mathbf{M}$ as

$$\frac{\partial \mathbf{M}}{\partial t} = \mathbf{M} \times \frac{\delta H}{\delta \mathbf{M}} + \mathbf{M} \times \boldsymbol{\mu}[\mathbf{M}] \times \frac{\delta E}{\delta \mathbf{M}},$$

thereby recovering exactly the Landau–Lifshitz–Gilbert equation (LLG) for magnetization dynamics (4) for the choice of magnetic mobility $\boldsymbol{\mu}[\mathbf{M}] = \mathbf{M}$, which arises from Kandrup's original choice of mobility, $\mu[f] = f$.

It is interesting to note that similar ideas for the extensions of Gilbert dissipation were recently suggested phenomenologically in [43].

5. Dissipative kinetic equation for moving particles with orientation

The kinetic approach for immobile oriented particles can be generalized to moving oriented particles. We use the energy-dissipation approach and generalize the formula (8) to more general Poisson bracket that involves both density and orientation. Interestingly enough, this

Poisson bracket was derived 25 years ago in Gibbons *et al* [11, 12] for Yang–Mills plasmas. We believe that we are the first to apply this bracket to dissipation in the setting of oriented particles. The modified Poisson bracket $\{\cdot,\cdot\}_1$ is defined as

$$\left\{f, \frac{\delta E}{\delta f}\right\}_1 = \left\{f, \frac{\delta E}{\delta f}\right\} + \left[f, \frac{\delta E}{\delta f}\right], \tag{15}$$

that is, it is a sum of a canonical Poisson bracket $\{\cdot,\cdot\}$ in single-particle position and canonical momentum and the rigid-body bracket $[\cdot,\cdot]$ in (12). For g belonging to the dual of a general Lie algebra $\mathfrak{g}$ (not necessarily $so(3)^*$), we can compute elements $\delta E/\delta g \in \mathfrak{g}$ and $\delta F/\delta g \in \mathfrak{g}$. We thus define a generalized rigid-body bracket as

$$[E, F] = \left\langle g, \left[\frac{\delta E}{\delta g}, \frac{\delta F}{\delta g}\right]_{LA}\right\rangle. \tag{16}$$

Here, we have used $[,]_{LA}$—the Lie algebra bracket in $\mathfrak{g}$. For this choice of the new bracket the quadratic form describing the dissipation (8) generalizes naturally to the anisotropic case as follows:

$$\frac{\mathrm{d}F}{\mathrm{d}t} = -\int \left\{\mu[f], \frac{\delta E}{\delta f}\right\}_1 \left\{f, \frac{\delta F}{\delta f}\right\}_1 \mathrm{d}\mathbf{x}. \tag{17}$$

Taking the moments of the anisotropic kinetic Vlasov equation following from (17) leads to a new kind of continuum dynamics naturally generalizing equation (1) to the case of anisotropic interaction. To simplify the formulae, we neglect the inertia of the particles. As mentioned in the introduction, this is a common assumption for friction-dominated systems. This assumption means neglecting the term $\{f, \delta H/\delta f\}$ in the left-hand side of (7). Thus we are left with the following equation which will form the core of further analysis,

$$\frac{\partial f}{\partial t} = \left\{f, \left\{\mu[f], \frac{\delta E}{\delta f}\right\}_1\right\}_1. \tag{18}$$

The remainder of this section follows the reasoning in [25], where the reader may find many more technical details and exposition of some related problems.

5.1. Landau–Lifshitz through the Smoluchowski approach

When dealing with kinetic theories, the kinetic moments are a well-established tool for deriving simplified continuum descriptions. However, in the case of anisotropic interactions, the kinetic moments $A_n = \int p^n f(q, p, g)\,\mathrm{d}p$ depend not only on the position coordinate, but also on the single-particle Lie algebra coordinate g. Thus, the moment equations differ from those found in the isotropic case, since they must include the terms which take into account the anisotropic behavior.

Moment dynamics has a Hamiltonian structure which is justified by the theorem that taking moments is a Poisson map. In fact, their dynamics is governed by the Kupershmidt–Manin bracket [13, 14]. This process can be transferred to the double-bracket formulation as follows. As in the Kupershmidt–Manin approach, the moments are dual to the variables $\beta_n(q, g)$, which are introduced by expanding the Hamiltonian function $h(q, p, g)$ as $h(q, p, g) = p^n\beta_n(q, g)$. The Lie algebra action is given by

$$\beta_n \cdot f = \left\{f, p^n\beta_n\right\}_1.$$

The dual action is defined by a star ($\star$) operator which is the symplectic equivalent of the diamond ($\diamond$) operation, as follows:

$$\langle f \star_n k, \beta_n\rangle := \langle f, \beta_n k\rangle = \langle f \star k, p^n\beta_n(q, g)\rangle = \left\langle \int p^n\{f, k\}_1\,\mathrm{d}p, \beta_n\right\rangle,$$

Thus, the star operator is defined explicitly for $k = p^m \alpha_m$ as

$$f \star_n k = \mathsf{ad}^*_{\alpha_m} A_{m+n-1} + \left\langle g, \left[\frac{\partial A_{m+n}}{\partial g}, \frac{\partial \alpha_m}{\partial g} \right] \right\rangle,$$

where the ad^* operator is the Kupershmidt–Manin Hamiltonian operator, see [13, 14]. We introduce the dissipative bracket by

$$\dot{F} = \{\{F, E\}\} = -\left\langle \mu[f] \star_n \frac{\delta E}{\partial f}, f \star_n \frac{\delta F}{\partial f} \right\rangle. \tag{19}$$

We truncate this sum at the simplest level, by taking $n = 0$. For higher order approximations, giving quite intricate formulae, see [25]. By using this evolution equation for an arbitrary functional F, the rate of change for zeroth moment A_0 is found to be

$$\frac{\partial A_0}{\partial t} = \left\langle g, \left[\frac{\partial A_0}{\partial g}, \frac{\partial \gamma_0}{\partial g} \right] \right\rangle,$$

where one defines $\gamma_0 := \mu[f] \star_0 \delta E / \delta f$, which is explicitly given by

$$\gamma_0 = \left\langle g, \left[\frac{\partial \mu_0}{\partial g}, \frac{\partial \beta_0}{\partial g} \right] \right\rangle.$$

Upon introducing the notation $\{\cdot, \cdot\}$ for the Lie–Poisson bracket on the Lie algebra $\mathfrak{g}$

$$\{k, h\} := \left\langle g, \left[\frac{\partial k}{\partial g}, \frac{\partial h}{\partial g} \right] \right\rangle,$$

we may write the equation for $\varphi = A_0$ in the double-bracket form,

$$\frac{\partial \varphi}{\partial t} = \left\{ \varphi, \left\{ \mu[\varphi], \frac{\delta E}{\delta \varphi} \right\} \right\}. \tag{20}$$

This is the purely dissipative moment equation corresponding to the Vlasov equation for the oriented particles (18). It is straightforward to see that the inclusion of the inertial part such as in equation (7) yields a moment equation of exactly the same form as equation (13)

$$\frac{\partial \varphi}{\partial t} + \left\{ \varphi, \frac{\delta H}{\delta \varphi} \right\} = \left\{ \varphi, \left\{ \mu[\varphi], \frac{\delta E}{\delta \varphi} \right\} \right\}. \tag{21}$$

We have now shown how to derive equation (13) from the kinetic approach by taking the zeroth moment. Next, one could continue by integrating over the microscopic magnetization $\boldsymbol{m}$ and thereby obtain the Landau–Lifshitz–Gilbert equation (4).

In the particular case $g = \boldsymbol{m} \in so(3)$ of interest to us for oriented-particle dynamics, the Lie–Poisson bracket reduces to the rigid-body bracket $\{\varphi, h\} := \boldsymbol{m} \cdot \nabla_m \varphi \times \nabla_m h$. The global Hamiltonian is written as $H[\varphi] = \int\int \varphi(q, \boldsymbol{m}) h(q, \boldsymbol{m}) \, \mathrm{d}q \, \mathrm{d}^3\boldsymbol{m}$ and an analogous expression holds for the dissipation energy $E[\varphi]$. The generalization to higher spatial dimensions is straightforward, since there are no derivatives in spatial coordinates in equation (21).

We next take moments with respect to $\boldsymbol{m}$. The particular physical case of magnetization density $\mathbf{M}(\boldsymbol{x}, t) := \int \boldsymbol{m} \varphi \, \mathrm{d}^3\boldsymbol{m}$ requires $H = E$. We assume that the single-particle energy h is linear in $\mathbf{m}$ since this assumption recovers the expression of the potential energy of a magnetic moment in a magnetic field. We consider only the dissipation terms in (13), i.e., we drop the second term on the left-hand side of that equation. Then, we obtain the rate of change of the energy $E[\varphi]$, as well as of an arbitrary functional $F[\varphi]$ in the quadratic form analogous to (8):

$$\frac{\mathrm{d}E}{\mathrm{d}t} = -\int \left[\mu[f], \frac{\delta E}{\delta f} \right]^2 \mathrm{d}\mathbf{x}, \qquad \frac{\mathrm{d}F}{\mathrm{d}t} = -\int \left[\mu[f], \frac{\delta E}{\delta f} \right] \left[f, \frac{\delta F}{\delta f} \right] \mathrm{d}\mathbf{x}. \tag{22}$$

The method of moments gives the equation for the magnetization density $\mathbf{M}$

$$\frac{\partial \mathbf{M}}{\partial t} = \mathbf{M} \times \frac{\delta H}{\delta \mathbf{M}} + \mathbf{M} \times \boldsymbol{\mu}[\mathbf{M}] \times \frac{\delta E}{\delta \mathbf{M}},$$

which recovers exactly the Landau–Lifshitz–Gilbert equation (LLG) for magnetization dynamics (4) for $\boldsymbol{\mu}[\mathbf{M}] = \mathbf{M}$, arising from Kandrup's original choice of mobility $\mu[f] = f$.

5.2. Dissipative moment dynamics: an alternative treatment

In this section, we extend the Kupershidt–Manin approach as in [11, 12] to generate the dynamics of moments with respect to both momentum p and charge g. The main technical complication is that the Lie algebras of physical interest (such as $\mathfrak{so}(3)$) are not one dimensional and in general are not Abelian. Thus, in the general case one needs to use a multi-index notation as in [32, 13]. We introduce multi-indices $\sigma := (\sigma_1, \sigma_2, \ldots, \sigma_N)$, with $\sigma_i \geqslant 0$, and define $g^\sigma := g_1^{\sigma_1} \ldots g_N^{\sigma_N}$, where $N = \dim(\mathfrak{g})$. Then, the moments are expressed as

$$A_{n\sigma}(q) := \int p^n g^\sigma f(q, p, g)\, \mathrm{d}p\, \mathrm{d}g.$$

This multi-dimensional treatment encumbers the calculations with technical complications. For the purposes of this section, we are primarily interested in the equations for ρ and G, so we restrict our considerations only to the moments of the form

$$A_{n,\nu} = \int p^n g_\nu f(q, p, g)\, \mathrm{d}p\, \mathrm{d}g \qquad \nu = 0, 1, \ldots, N.$$

Here we define $g_0 = 1$ and $g_a = \langle g, \mathbf{e}_a \rangle$ where $\mathbf{e}_a$ is a basis of the Lie algebra and $\langle g_b \mathbf{e}^b, \mathbf{e}_a \rangle = g_a \in \mathbb{R}$ represents the result of the pairing $\langle \cdot, \cdot \rangle$ between an element of the Lie algebra basis and an element of the dual Lie algebra. We write the single-particle Hamiltonian as $h = \delta H/\delta f = p^n g_\nu \delta H/\delta A_{n,\nu} =: p^n g_\nu \beta_n^\nu(q)$, which means that we employ the following assumption.

Assumption 5.1. *The single-particle Hamiltonian $h = \delta H/\delta f$ is linear in g and can be expressed as*

$$h(q, p, g) = p^n \psi_n(q) + p^n \langle g, \overline{\psi}_n(q) \rangle,$$

where $\psi_n(q) \in \mathbb{R}$ is a real scalar function and $\overline{\psi}_n(q) \in \mathbb{R} \times \mathfrak{g}$ is a real Lie-algebra-valued function.

Dual Lie algebra action. The action of β_n^ν on f is defined as

$$\beta_n^\nu \cdot f = \left\{ p^n g_\nu \beta_n^\nu, f \right\}_1 \qquad \text{(no sum)}.$$

The dual of this action is denoted by $(\star_{n,\nu})$. It may be computed analogously to (10) and found to be

$$\begin{aligned} f \star_{n,\nu} k &= \iint p^n g_\nu \left\{ f, k \right\}_1 \mathrm{d}p\, \mathrm{d}g \\ &= \int g_\nu g_\sigma \mathsf{ad}^*_{\alpha_m^\sigma} A_{m+n-1}\, \mathrm{d}g + \int g_\nu \left\langle g, \left[\frac{\partial A_{m+n}}{\partial g}, \frac{\partial (g_\sigma \alpha_m^\sigma)}{\partial g} \right] \right\rangle \mathrm{d}g \\ &= \mathsf{ad}^*_{\alpha_m^\sigma} \int g_\nu g_\sigma A_{m+n-1}\, \mathrm{d}g + \int g_\nu \left\langle g, \left[\frac{\partial A_{m+n}}{\partial g}, \frac{\partial (g_a \alpha_m^a)}{\partial g} \right] \right\rangle \mathrm{d}g. \end{aligned}$$

Here, $k = p^m g_\sigma \alpha_m^\sigma(q)$ and we have used the definition of the moment

$$A_n(q, g) = \int p^n f(q, p, g)\, \mathrm{d}p.$$

Evolution equation. Having characterized the dual Lie algebra action, we may now write the evolution equation for an arbitrary functional F in terms of the dissipative bracket as follows:

$$\dot{F} = \{\{F, E\}\} = -\left\langle\!\!\left\langle \left(\mu[f]\star_{n,\nu}\frac{\delta E}{\partial f}\right)^{\sharp}, f\star_{n,\nu}\frac{\delta F}{\partial f}\right\rangle\!\!\right\rangle, \tag{23}$$

where the pairing $\langle\!\langle\cdot,\cdot\rangle\!\rangle$ is given by integration over the spatial coordinate q. Now we fix $m = 0, n = 1$. The equation for the evolution of $F = A_{0,\lambda} := \int g_\lambda A_0 \,\mathrm{d}g\,\mathrm{d}p$ is found from (23) to be

$$\frac{\partial A_{0,\lambda}}{\partial t} = \frac{\partial}{\partial q}\left(\gamma_{1,\nu}^{\sharp}\int g_\nu g_\lambda A_0\,\mathrm{d}g\right) + \int g_\lambda\left\langle g, \left(\left[\frac{\partial A_1}{\partial g}, \frac{\partial\left(g_a\gamma_{1,a}^{\sharp}\right)}{\partial g}\right] + \left[\frac{\partial A_0}{\partial g}, \frac{\partial\left(g_a\gamma_{0,a}^{\sharp}\right)}{\partial g}\right]\right)\right\rangle \mathrm{d}g, \tag{24}$$

where we have defined the analogues of Darcy's velocities:

$$\gamma_{0,\nu} := \mu[f]\star_{0,\nu}\frac{\delta E}{\delta f} = \int g_\nu\left\langle g, \left[\frac{\partial\widetilde{\mu}_k}{\partial g}, \frac{\partial\left(g_a\beta_k^a\right)}{\partial g}\right]\right\rangle \mathrm{d}g = \int g_\nu\left\langle g, \left[\frac{\partial\widetilde{\mu}_0}{\partial g}, \frac{\partial\left(g_a\beta_0^a\right)}{\partial g}\right]\right\rangle \mathrm{d}g,$$

and

$$\gamma_{1,\nu} := \mu[f]\star_{1,\nu}\frac{\delta E}{\delta f} = \frac{\partial\beta_0^\sigma}{\partial q}\int g_\nu g_\sigma\widetilde{\mu}_0\,\mathrm{d}g + \int g_\nu\left\langle g, \left[\frac{\partial\widetilde{\mu}_1}{\partial g}, \frac{\partial\left(g_a\beta_0^a\right)}{\partial g}\right]\right\rangle \mathrm{d}g,$$

with $\widetilde{\mu}_k := \int p^k f\,\mathrm{d}p$. Here we have assumed that the energy functional E depends only on $A_{0,\lambda}$ (recall that $\beta_n^\lambda := \delta E/\delta A_{n,\lambda}$), so that we may fix $k = 0$ in the second line. At this point, we further simplify the treatment by discarding all terms in $\gamma_{1,a}$, that is we truncate the summations in equation (24) to consider only terms in $\gamma_{0,0}, \gamma_{0,a}$ and $\gamma_{1,0}$. With this simplification, equation (24) becomes

$$\frac{\partial A_{0,\lambda}}{\partial t} = \frac{\partial}{\partial q}\left(\gamma_{1,0}\int g_\lambda A_0\,\mathrm{d}g\right) + \int g_\lambda\left\langle g, \left(\left[\frac{\partial A_0}{\partial g}, \frac{\partial\left(g_a\gamma_{0,a}^{\sharp}\right)}{\partial g}\right]\right)\right\rangle \mathrm{d}g, \tag{25}$$

and the expression for $\gamma_{1,0}$ is

$$\gamma_{1,0} := \mu[f]\star_{1,0}\frac{\delta E}{\delta f} = \frac{\partial\beta_0^\sigma}{\partial q}\int g_\sigma\widetilde{\mu}_0\,\mathrm{d}g.$$

Let us now define the *dynamic quantities*

$$\rho = \int f\,\mathrm{d}g\,\mathrm{d}p, \qquad G = \int gf\,\mathrm{d}g\,\mathrm{d}p,$$

and corresponding *mobilities*

$$\mu_\rho = \int \mu[f]\,\mathrm{d}g\,\mathrm{d}p, \qquad \mu_G = \int g\mu[f]\,\mathrm{d}g\,\mathrm{d}p.$$

In terms of these quantities, we may write the following.

Theorem 5.2. *The moment equations for ρ and G are given by*

$$\frac{\partial\rho}{\partial t} = \frac{\partial}{\partial q}\left(\rho\left(\mu_\rho\frac{\partial}{\partial q}\frac{\delta E}{\delta\rho} + \left\langle\mu_G, \frac{\partial}{\partial q}\frac{\delta E}{\delta G}\right\rangle\right)\right) \tag{26}$$

and

$$\frac{\partial G}{\partial t} = \frac{\partial}{\partial q}\left(G\left(\mu_\rho\frac{\partial}{\partial q}\frac{\delta E}{\delta\rho} + \left\langle\mu_G, \frac{\partial}{\partial q}\frac{\delta E}{\delta G}\right\rangle\right)\right) + \mathrm{ad}^*_{\left(\mathrm{ad}^*_{\frac{\delta E}{\delta G}}\mu_G\right)^\sharp}G. \tag{27}$$

Remark 5.3. Similar equations (under the name of geometric order parameter equations) were derived via a general geometric considerations in [23]. The equations presented here reduce to those for the case of commutative Lie algebras.

Remark 5.4. Although in this section the underlying space where particles undergo their motion is assumed to be one dimensional, the extension to higher spatial dimensions is trivial: since the Lie derivative of a density is given by the divergence term in spatial coordinate $\mathbf{q}$, we need to substitute div and grad instead of one-dimensional derivatives with respect to $\mathbf{q}$. See (28), (29) immediately below for an explicitly computed particular case.

6. Self-organization dynamics of moving magnets

We are now ready to write out explicit equations for the motion of magnets in $d = 1, 2$ or 3 dimensions. In this case $G = \mathbf{M}(x) \in \mathbb{R}^3$—average magnetization, $\mathrm{ad}_{\mathbf{v}}\mathbf{w} = \mathbf{v} \times \mathbf{w}$ and $\mathrm{ad}^*_{\mathbf{v}}\mathbf{w} = -\mathbf{v} \times \mathbf{w}$, and the Lie algebra pairing is represented by the dot product of vectors in $\mathbb{R}^3$. Therefore, the equations for $(\rho, \mathbf{M})$ are obtained directly from (26), (27) and are written as follows:

$$\frac{\partial \rho}{\partial t} = \mathrm{div}\left(\rho\left(\mu_\rho \nabla \frac{\delta E}{\delta \rho} + \boldsymbol{\mu}_{\mathbf{M}} \cdot \nabla \frac{\delta E}{\delta \mathbf{M}}\right)\right), \tag{28}$$

and

$$\frac{\partial \mathbf{M}}{\partial t} = \mathrm{div}\left(\mathbf{M} \otimes \left(\mu_\rho \nabla \frac{\delta E}{\delta \rho} + \boldsymbol{\mu}_{\mathbf{M}} \cdot \nabla \frac{\delta E}{\delta \mathbf{M}}\right)\right) + \mathbf{M} \times \boldsymbol{\mu}_{\mathbf{M}} \times \frac{\delta E}{\delta \mathbf{M}}. \tag{29}$$

This is the generalization of the Landau–Lifshitz–Gilbert and Debye–Hückel equations we have sought. The main consequence of equations (29) is that they allow single-particle solutions of the form

$$\begin{aligned} \rho(\boldsymbol{x}, t) &= w_\rho(t)\delta(\boldsymbol{x} - \boldsymbol{Q}(t)), \\ \mathbf{M}(\boldsymbol{x}, t) &= \boldsymbol{w}_{\mathbf{M}}(t)\delta(\boldsymbol{x} - \boldsymbol{Q}(t)). \end{aligned} \tag{30}$$

where w_ρ, $\boldsymbol{w}_{\mathbf{M}}$ and $\boldsymbol{Q}$ undergo the following dynamics:

$$\dot{w}_\rho = 0, \qquad \dot{\boldsymbol{w}}_{\mathbf{M}} = \left(\boldsymbol{w}_{\mathbf{M}} \times \boldsymbol{\mu}_{\mathbf{M}} \times \frac{\delta E}{\delta \mathbf{M}}\right)_{\boldsymbol{x}=\boldsymbol{Q}}, \qquad \dot{\boldsymbol{Q}} = -\left(\mu_\rho \nabla \frac{\delta E}{\delta \rho} + \boldsymbol{\mu}_{\mathbf{M}} \cdot \nabla \frac{\delta E}{\delta \mathbf{M}}\right)_{\boldsymbol{x}=\boldsymbol{Q}}.$$

These solutions have an important physical meaning, since they represent particles that aggregate and align. This phenomenon is of fundamental importance in the theory of anisotropic self-assembly. There are special cases where these solutions emerge spontaneously from any confined initial distribution. These behavior depends on the particular choice of mobilities and energy functionals. A typical result of simulations is presented in figure 1. Starting with a random distribution in one dimension, we see the formation of sharp peaks in magnetization $\mathbf{M}$ (left figure) and density ρ (color code on the left and plot on the right), corresponding to the δ-functions.

7. Moving dissipative oriented curves: new variables in geometric dynamics

The structure of singular solutions allows us an interesting geometric generalization, namely a possibility for singular solutions to be concentrated on a one-dimensional manifold (a curve) in the two- or three-dimensional space. This will give an interesting addition to the theory of exact geometric rods [40], as our equations describe the *dissipative* motion of a curve.

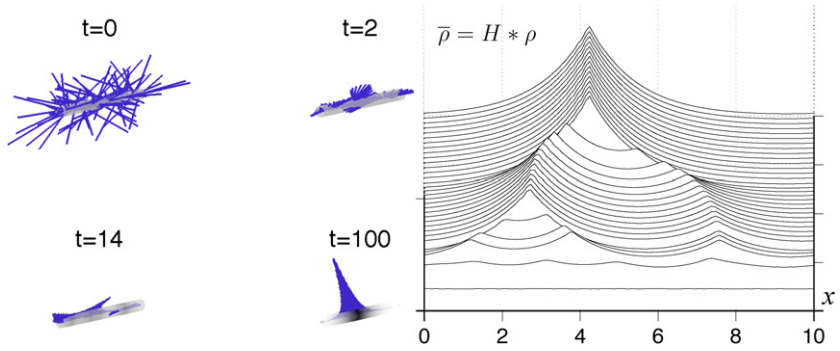

Figure 1. Left: a typical example of formation of *orientons* in a $d = 1$ dimensional simulation. The color code on the cylinder denotes the local *averaged* density $\overline{\rho} = H * \rho$ for a Helmholtz kernel $H = \mathrm{e}^{-|x|}$: black is the maximum density while white is $\overline{\rho} = 0$. Purple lines denote the three-dimensional vector $\overline{\mathbf{M}} = H * \mathbf{M}$. The formation of sharp peaks in averaged quantities corresponds to the formation of δ-functions in (28), (29) according to (30). Averaged quantities were chosen to avoid the necessity to represent δ-functions. Right: the corresponding waterfall plot for evolution of averaged density $\overline{\rho} = H * \rho$. Horizontal coordinate is space. Sharp peaks correspond to the formation of δ-function singularities in the density variable ρ.

Formally, we extend equations (30) and assume that the solution is concentrated on a curve in space $\mathbf{r} = \mathbf{Q}(s, t)$, where s is the arclength. Then, we are interested in the solutions of the form

$$\begin{aligned} \rho(\boldsymbol{x}, t) &= \int w_\rho(s, t)\delta(\boldsymbol{x} - \boldsymbol{Q}(s, t))ds \\ \mathbf{M}(\boldsymbol{x}, t) &= \int \boldsymbol{w}_\mathbf{M}(s, t)\delta(\boldsymbol{x} - \boldsymbol{Q}(s, t))ds. \end{aligned} \tag{31}$$

Multiplying each equation (28), (29) by a test function and integrating produces the following equations of motion:

$$\frac{\partial}{\partial t} w_\rho(s, t) = 0, \tag{32}$$

$$\frac{\partial}{\partial t} \boldsymbol{w}_\mathbf{M}(s, t) = \boldsymbol{w}_\mathbf{M} \times \boldsymbol{\mu}_\mathbf{M}(\boldsymbol{Q}(s, t)) \times \frac{\delta E}{\delta \mathbf{M}}(\boldsymbol{Q}(s, t)), \tag{33}$$

$$\frac{\partial}{\partial t} \boldsymbol{Q}(s, t) = \mu_\rho(s, t)\nabla \frac{\delta E}{\delta \rho}(\boldsymbol{Q}(s, t)) + \boldsymbol{\mu}_\mathbf{M}(s, t)\nabla \frac{\delta E}{\delta \mathbf{M}}(\boldsymbol{Q}(s, t)). \tag{34}$$

In the simplest case of a binary energy functional,

$$E = \frac{1}{2} \int \rho(\mathbf{x})\rho(\mathbf{x}')G_\rho(\mathbf{x} - \mathbf{x}') + \mathbf{M}(\mathbf{x})\mathbf{M}(\mathbf{x}')G_\mathbf{M}(\mathbf{x} - \mathbf{x}')\, \mathrm{d}^3x\, \mathrm{d}^3x', \tag{35}$$

where $G_\mathbf{M}$ is assumed to be a scalar function, equation (34) assumes an especially simple and elegant shape (see also [24]):

$$\begin{aligned} \frac{\partial}{\partial t} \boldsymbol{Q}(s, t) = \int & \mu_\rho(s, t)\rho(s', t)\nabla G_\rho(\boldsymbol{Q}(s, t), \boldsymbol{Q}(s', t)) \\ & + \boldsymbol{\mu}_\mathbf{M}(s, t) \cdot \mathbf{M}(s', t)\nabla G_\mathbf{M}(\boldsymbol{Q}(s, t), \boldsymbol{Q}(s', t))\, \mathrm{d}s'. \end{aligned} \tag{36}$$

To illustrate the concepts developed above, we perform a simulation of the spatio-temporal evolution for two oriented curves, having the simplest energy dependence given by (35). In the

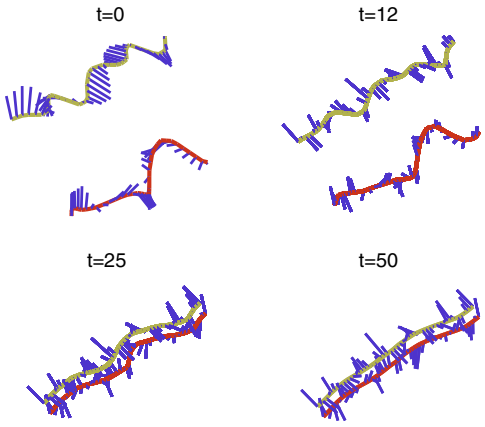

Figure 2. An example of two oriented curves (red and green) attracting each other and unwinding at the same time. The blue vectors illustrate the vector $\mathbf{M} \in so(3)$ at each point on the curve. Time scale is arbitrary.

future, we shall consider more sophisticated models of energy using the technique developed in (49) below. In computer simulations presented in figure 2, we assumed centrally symmetric Lennard–Jones potential for the density interaction and the Helmholtzian $G_M(\mathbf{x}) = \exp(-|\mathbf{x}|)$ for the orientation part of energy. Initially, the curves are far away from each other and the $\mathbf{M}$ values on the curves are unrelated. Eventually, the curves collapse to two parallel lines and the $\mathbf{M}$ vectors on both curves align.

8. Orientation-dependent interaction energies: geometric considerations

Energy (35) provides insight, but it is too simple to describe many interesting physical phenomena, for example, dynamics of assembly of biologically relevant particles into curves like DNA. The energy of these particles depends on the position $\mathbf{x}$ and orientation $\Lambda(\mathbf{x})$ of a frame at a point $\mathbf{x}$, and the *relative* distances and orientations with respect to all other points $\mathbf{x}'$. We are thus compelled to deal with more interesting energies reflecting this physical fact, and this will lead us to some interesting mathematical consequences. The technical question here is how to compute $\delta E/\delta \mathbf{M}$, if the energy is given in terms of Λ. Of particular interest to us is the so-called anisotropic Lennard–Jones potential that has been developed in [39] and has been subsequently applied to produce self-organization of anisotropic particles into the shape of a double helix [10]. The idea of this method is the following.

Consider two ellipsoids with the geometric centers at $\mathbf{x}$ and $\mathbf{x}'$ and orientation with respect to the fixed frame $\Lambda(\mathbf{x})$ and $\Lambda(\mathbf{x}')$, respectively. The method computes the distance $d(\mathbf{x}, \mathbf{x}', \Lambda(\mathbf{x}), \Lambda(\mathbf{x}'))$ between ellipsoidal surfaces along the direction of $\mathbf{x} - \mathbf{x}'$. This is close to the minimal distance between the ellipsoids, but it is easier to compute. In principle, to make the depth of the potential well different for attracting and repulsive potential, one can consider two distances $d = d_1$ and $d = d_2$, corresponding to the attractive and repulsive parts of the ellipsoids. The distances d_1 and d_2 are defined as $d_i = \sigma_0 + |\mathbf{x} - \mathbf{x}'| + f_i(\Lambda(\mathbf{x}, \lambda\mathbf{x}'))$, where σ_0 is a given constant and f_i are some (rather complex) functions. One then takes the potential to be the Lennard–Jones potential of the modified distances

$$U\{d(\mathbf{x}, \mathbf{x}', \Lambda(\mathbf{x}), \Lambda(\mathbf{x}'))\} = 4\epsilon_0 \left[\left(\frac{\sigma_0}{d_1} \right)^{12} - \left(\frac{\sigma_0}{d_2} \right)^{6} \right]. \tag{37}$$

An important feature of this potential that has not been noted in previous works is its invariance with respect to $SO(3)$ rotations about each point on the curve. Thus, the energy functional may be written as

$$E = \frac{1}{2}\int \rho(\mathbf{x})\rho(\mathbf{x}')U(\mathbf{x}, \mathbf{x}', \Lambda(\mathbf{x}), \Lambda(\mathbf{x}'))\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}', \tag{38}$$

where U is some scalar function of its arguments. This energy is still *binary*, i.e. it is a direct sum of pairwise interaction of all particles, which is known to be a rather crude approximation for real systems. However, we believe it is important to first understand this $SO(3)$-invariant energy. Later, the equations of motion for more general energies may be obtained by direct generalization. Invariance with respect to the rotation group requires that the energy of particle interaction assumes the following form:

$$E = \frac{1}{2}\int \rho(\mathbf{x})\rho(\mathbf{x}')U(|\mathbf{x} - \mathbf{x}'|, \xi(\mathbf{x}, \mathbf{x}'))\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}', \tag{39}$$

where we have defined

$$\xi(\mathbf{x}, \mathbf{x}') = \Lambda(\mathbf{x})^{-1}\Lambda(\mathbf{x}') \in SO(3). \tag{40}$$

Remark 8.1. Note that we have assumed that the energy does not depend directly on a Lie algebra element $\widehat{\mathbf{M}} = \Lambda^{-1}\nabla\Lambda$. That means, in particular, that elastic energy caused by particle motion is not included. The introduction of elastic energy complicates the equations and will be considered in future work.

Now, we need to compute $\delta E/\delta\Lambda$. We proceed as follows. Define $\Sigma(\mathbf{x}) = \Lambda^{-1}(\mathbf{x})\delta\Lambda(\mathbf{x}) \in so(3)$. Then, note that

$$\begin{aligned}
\delta\xi &= \delta(\Lambda^{-1}(\mathbf{x})\Lambda(\mathbf{x}')) \\
&= -\Lambda^{-1}(\mathbf{x})\delta\Lambda(\mathbf{x})\Lambda^{-1}(\mathbf{x})\Lambda(\mathbf{x}') + \Lambda^{-1}(\mathbf{x})\delta\Lambda(\mathbf{x}') \\
&= -\Sigma(\mathbf{x})\xi(\mathbf{x}, \mathbf{x}') + \Lambda^{-1}(\mathbf{x})\Lambda(\mathbf{x}')\Lambda^{-1}(\mathbf{x}')\delta\Lambda(\mathbf{x}') \\
&= -\Sigma(\mathbf{x})\xi(\mathbf{x}, \mathbf{x}') + \xi(\mathbf{x}, \mathbf{x}')\Sigma(\mathbf{x}'),
\end{aligned} \tag{41}$$

since $\xi = \Lambda^{-1}(\mathbf{x})\Lambda(\mathbf{x}') \in SO(3)$. Thus,

$$\begin{aligned}
\delta E &= \int \rho(\mathbf{x})\rho(\mathbf{x}')\mathrm{tr}\left(\left(\frac{\partial U}{\partial\xi}(\mathbf{x}, \mathbf{x}')\right)^T \{-\Sigma(\mathbf{x})\xi(\mathbf{x}, \mathbf{x}') + \xi(\mathbf{x}, \mathbf{x}')\Sigma(\mathbf{x}')\}\right)\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}' \\
&= \int \rho(\mathbf{x})\rho(\mathbf{x}')\mathrm{tr}\left(-\left(\frac{\partial U}{\partial\xi}(\mathbf{x}, \mathbf{x}')\xi(\mathbf{x}, \mathbf{x}')^T\right)^T \Sigma(\mathbf{x})\right)\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}' \\
&\quad + \int \rho(\mathbf{x})\rho(\mathbf{x}')\mathrm{tr}\left(\left(\xi(\mathbf{x}, \mathbf{x}')^T\frac{\partial U}{\partial\xi}(\mathbf{x}, \mathbf{x}')\right)^T \Sigma(\mathbf{x}')\right)\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}'.
\end{aligned} \tag{42}$$

In the last term, $\mathbf{x}$ and $\mathbf{x}'$ were exchanged to make the variation $\Sigma(\mathbf{x}')$ a function of $\mathbf{x}$. When making this exchange, we must remember that

$$\xi(\mathbf{x}, \mathbf{x}') = \Lambda(\mathbf{x})^{-1}\Lambda(\mathbf{x}') = \xi^{-1}(\mathbf{x}', \mathbf{x}) = \xi^T(\mathbf{x}', \mathbf{x})$$

and similarly,

$$\frac{\partial U}{\partial\xi}(\mathbf{x}, \mathbf{x}') = \left(\frac{\partial U}{\partial\xi}(\mathbf{x}', \mathbf{x})\right)^T.$$

Consequently, we find

$$\delta E = \int \rho(\mathbf{x})\rho(\mathbf{x}')\mathrm{tr}\left(-\left(\frac{\partial U}{\partial \xi}(\mathbf{x},\mathbf{x}')\xi(\mathbf{x},\mathbf{x}')^T\right)^T \Sigma(\mathbf{x})\right) + \int \rho(\mathbf{x})\rho(\mathbf{x}')\mathrm{tr}\left(\left(\xi(\mathbf{x},\mathbf{x}')\left(\frac{\partial U}{\partial \xi}(\mathbf{x},\mathbf{x}')\right)^T\right)^T \Sigma(\mathbf{x})\right)\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}'.$$

Thus, collecting terms leads to

$$\delta E = \int \rho(\mathbf{x})\rho(\mathbf{x}')\left\langle -\frac{\partial U}{\partial \xi}(\mathbf{x},\mathbf{x}')\xi(\mathbf{x},\mathbf{x}')^T + \xi(\mathbf{x},\mathbf{x}')\left(\frac{\partial U}{\partial \xi}(\mathbf{x},\mathbf{x}')\right)^T, \Sigma(\mathbf{x})\right\rangle \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}'.$$

If we now turn from the variations in Σ to variations in Λ, we find Λ in front of the integral, and the final formula for the variation of energy is thus

$$\frac{\delta E}{\delta \Lambda} = \Lambda(\mathbf{x})\rho(\mathbf{x})\int \rho(\mathbf{x}')\left\{-\frac{\partial U}{\partial \xi}(\mathbf{x},\mathbf{x}')\xi^T(\mathbf{x},\mathbf{x}') + \xi(\mathbf{x},\mathbf{x}')\left(\frac{\partial U}{\partial \xi}(\mathbf{x},\mathbf{x}')\right)^T\right\}\mathrm{d}\mathbf{x}'. \tag{43}$$

We have computed the variations with respect to Λ. We are not finished yet, as the equations of motion of a string are formulated on the Lie algebra, not the tangent bundle of the Lie group. Thus, we need to connect $\delta E/\delta\Lambda$ to $\delta E/\delta\widehat{\mathbf{M}}$.[6] To do that, we use the definition of the left-invariant tangent space at the identity,

$$\widehat{\mathbf{M}}_i = \Lambda^{-1}\frac{\partial \Lambda}{\partial x^i} \in so(3), \qquad i = 1, 2, \ldots, d, \tag{44}$$

where x^i is the ith coordinate in space. The Lie algebra element is then a 'vector' of d antisymmetric matrices, where d is the dimension of the space. We have, by the usual change of variables (summation over repeated indices is assumed),

$$\delta E = \left\langle \frac{\delta E}{\delta \Lambda}, \delta\Lambda \right\rangle = \left\langle \frac{\delta E}{\delta \widehat{\mathbf{M}}_i}, \delta\widehat{\mathbf{M}}_i \right\rangle, \tag{45}$$

where $\delta E/\delta\widehat{\mathbf{M}} \in so(3)^*$. Denote again $\Sigma(\mathbf{x}) = \Lambda^{-1}(\mathbf{x})\delta\Lambda(\mathbf{x}) \in so(3)$. Then,

$$\delta\widehat{\mathbf{M}}_i = -\Sigma\widehat{\mathbf{M}}_i + \Lambda^{-1}\frac{\partial}{\partial x^i}\delta\Lambda.$$

Thus, (45) becomes

$$\left\langle \frac{\delta E}{\delta \Lambda}, \delta\Lambda \right\rangle = \left\langle \frac{\delta E}{\delta \widehat{\mathbf{M}}_i}, -\Sigma\widehat{\mathbf{M}}_i + \Lambda^{-1}\frac{\partial}{\partial x^i}\Lambda\Sigma \right\rangle = \left\langle \frac{\delta E}{\delta \widehat{\mathbf{M}}_i}, \left[\widehat{\mathbf{M}}_i, \Sigma\right] \right\rangle - \left\langle \frac{\partial}{\partial x^i}\frac{\delta E}{\delta \widehat{\mathbf{M}}_i}, \Sigma \right\rangle. \tag{46}$$

Remembering that $\Sigma = \Lambda^{-1}\delta\Lambda$ and setting Λ using the pairing properties $\langle a, \Lambda b\rangle = \langle \Lambda^T a, b\rangle$ leads to the following expression (as $(\Lambda^{-1})^T = \Lambda$):

$$\frac{\delta E}{\delta \Lambda} = \Lambda\left(\mathrm{ad}^*_{\widehat{\mathbf{M}}_i}\frac{\delta E}{\delta \widehat{\mathbf{M}}_i} - \frac{\partial}{\partial x^i}\frac{\delta E}{\delta \widehat{\mathbf{M}}_i}\right). \tag{47}$$

This can be written in a familiar way in terms of the vector product in $\mathbb{R}^3$ as

$$\frac{\delta E}{\delta \Lambda} = -\Lambda\left(\mathbf{M}_i \times \frac{\delta E}{\delta \mathbf{M}_i} + \frac{\partial}{\partial x^i}\frac{\delta E}{\delta \mathbf{M}_i}\right)\widehat{\ }, \tag{48}$$

which is an extension of the formula (6.18d) of [40].

[6] Here, the hat denotes the usual isomorphism between vectors in $\mathbb{R}^3$ and elements of Lie algebra $so(3)$, so $\widehat{\mathbf{M}} \in so(3)$ and $\mathbf{M} \in \mathbb{R}^3$.

Combining equations (48) and (43) yields an auxiliary equation for $\delta E/\delta \mathbf{M}$ that is valid for any value of $\mathbf{x}$:

$$\left(\mathbf{M}_i(\mathbf{x}) \times \frac{\delta E}{\delta \mathbf{M}_i}(\mathbf{x}) + \frac{\partial}{\partial x^i}\frac{\delta E}{\delta \mathbf{M}_i}(\mathbf{x})\right)^{\widehat{}} = -\rho(\mathbf{x}) \int \rho(\mathbf{x}')\left\{-\frac{\partial U}{\partial \xi}(\mathbf{x},\mathbf{x}')\xi(\mathbf{x},\mathbf{x}')^T + \xi(\mathbf{x},\mathbf{x}')\left(\frac{\partial U}{\partial \xi}(\mathbf{x},\mathbf{x}')\right)^T\right\} \mathrm{d}\mathbf{x}', \tag{49}$$

where, again, $\xi(\mathbf{x},\mathbf{x}') := \Lambda^{-1}(\mathbf{x})\Lambda(\mathbf{x}') \in SO(3)$. The left-hand side of this equation is the $so(3)^*$-valued covariant divergence of the $so(3)^*$ vector $\delta E/\delta \mathbf{M}_i$, which is also a 3-by-3 antisymmetric matrix for each $i = 1, 2, \ldots, d$. Likewise, the expression in curly brackets is an antisymmetric 3-by-3 matrix, as one may verify by taking the transpose. Thus equation (49) is consistent. In fact, equation (49) is reminiscent of the Yang–Mills–Gauss Law for an $so(3)^*$-valued gauge charge. A similar equation appears in the gauge-theoretical formulation of the dynamical equations for a spin-glass [19]. The gauge freedom remaining in equation (49) is removed by noting that $\mathbf{M}_i$ defined in (44) is a pure gauge field. Consequently, the connection associated with the $so(3)$-valued covariant divergence in (49) must have no curvature. Hence, for any i, j, we find the following consistency conditions:

$$\frac{\partial \widehat{\mathbf{M}}_i}{\partial x^j} - \frac{\partial \widehat{\mathbf{M}}_j}{\partial x^i} = [\widehat{\mathbf{M}}_i, \widehat{\mathbf{M}}_j] = \widehat{\mathbf{M}}_i\widehat{\mathbf{M}}_j - \widehat{\mathbf{M}}_j\widehat{\mathbf{M}}_i, \tag{50}$$

which close the system (49).

Remark 8.2. It is interesting to note the similarity between the variable $\xi = \Lambda^{-1}(\mathbf{x})\Lambda(\mathbf{x}')$ and its time analogue $\Lambda(t)^{-1}\Lambda(t+\Delta)$, which is commonly used in discrete-time Moser–Veselov integrators [36] and their extensions [9]. Further study of the geometric nature of (49) appears intriguing and will be undertaken in the future.

Let us see how (49) reduces on the singular solutions (31). Assuming that the potential U is such that $\partial U/\partial \xi$ remains finite on the singular solutions, we substitute (31) into (43) to find

$$\frac{\delta E}{\delta \Lambda}(\mathbf{x}) = \Lambda(\mathbf{x}) w_\rho(s,t)\delta(\mathbf{x} - \boldsymbol{Q}(s,t)) \times \int w_\rho(s',t)\left\{-\frac{\partial U}{\partial \xi}(s,s')\xi^T(s,s') + \xi(s,s')\left(\frac{\partial U}{\partial \xi}(s,s')\right)^T\right\} \mathrm{d}\mathbf{x}', \tag{51}$$

where we have denoted

$$\xi(s,s') := \xi(\boldsymbol{Q}(s,t), \boldsymbol{Q}(s',t)) \qquad \text{and} \qquad \frac{\partial U}{\partial \xi}(s,s') := \frac{\partial U}{\partial \xi}(\boldsymbol{Q}(s,t), \boldsymbol{Q}(s',t)).$$

Upon multiplying each side of the equation (49) by an arbitrary function $\phi(\mathbf{x})$, integrating over the whole space and equating the coefficients of $\phi(\boldsymbol{Q}(s,t))$, we obtain the following relation:

$$\left(\boldsymbol{w}_{\mathbf{M}}(s) \times \frac{\delta E}{\delta \mathbf{M}}(s) + \frac{\partial}{\partial s}\frac{\delta E}{\delta \mathbf{M}}(s)\right)^{\widehat{}} = -w_\rho(s) \int w_\rho(s')\left\{-\frac{\partial U}{\partial \xi}(s,s')\xi(s,s')^T + \xi(s,s')\left(\frac{\partial U}{\partial \xi}(s,s')\right)^T\right\} \mathrm{d}s'. \tag{52}$$

This is the equation for the computation of the variations $\delta E/\delta \mathbf{M}$ on the curve that we have sought. The analogue for curves of the consistency condition (50) then closes the system. Future work will explore its dynamics and numerical solutions.

9. Conclusions

In this paper, we explained the derivation of continuum equations for dissipation using the moment approach in kinetic (Vlasov) equations. We showed how to introduce dissipation in Vlasov equations based on a geometric generalization of the Darcy's law of motion (force being proportional to velocity). We derived the continuum equations of motions in general settings and then formulated those equations for the particular case of self-organization of magnetic particles. We showed the existence and spontaneous emergence of generalized solutions concentrated on delta functions. We also showed that the equations possess singular solutions concentrated on one-dimensional manifolds (curves) and derived equations of motion for these curves.

Of particular interest for future work are two questions. The first question is: can solutions defining singular curves appear from random initial conditions in two or three dimensions? The positive answer to this question would demonstrate the possibility of controlling magnetic self-assembly of dispersed particles into *magnetic strings*, which would be very interesting technologically.

The second question is: can both inertial and dissipative terms be incorporated consistently into the theory of geometrically exact rods? Hopefully, this can be accomplished by starting with the dissipative Vlasov equation containing the inertia terms, repeating the procedure of [11, 12] keeping the momentum term and closing the system using either truncation or the cold plasma approximation. An interesting task would be to compare the resulting dissipative equations with those of the geometrically exact rods in the absence of dissipation [40].

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References

[1] Barth J V, Costantini G and Kern K 2005 Engineering atomic and molecular nano-structures at surfaces *Nature* **437** 671–9
[2] Batchelor G K 2000 *An Introduction to Fluid Dynamics* (Cambridge: Cambridge University Press)
[3] Bloch A M, Brockett R W and Ratiu T S 1992 Completely integrable gradient flows *Commun. Math. Phys.* **147** 57–74
[4] Bloch A M, Krishnaprasad P S, Marsden J E and Ratiu T S 1996 The Euler–Poincaré equations and double-bracket dissipation *Commun. Math. Phys.* **175** 1–42
[5] Bloembergen N 1950 On the ferromagnetic resonance in nickel and supermalloy *Phys. Rev.* **78** 572–80
[6] Chavanis P H, Laurençot P and Lemou M 2004 Chapman–Enskog derivation of the generalized Smoluchowski equation *Physica* A **341** 145–64
[7] Codrington R S, Olds J D and Torrey H C 1954 Paramagnetic resonance in organic free radicals at low fields *Phys. Rev.* **95** 607–8

[8] Debye P and Hückel E 1924 The interionic attraction theory of deviations from ideal behavior in solution II *Z. Phys.* 25–97
[9] Dixon M 2007 Geometric integrators for continuum mechanics *PhD Thesis* Imperial College, London
[10] Fejer S N and Wales D J 2007 Helix self-assembly from anisotropic particles *Phys. Rev. Lett.* **99** 086106
[11] Gibbons J, Holm D D and Kupershmidt B A 1982 Gauge-invariant Poisson brackets for chromohydrodynamics *Phys. Lett.* A **90** 281–3
[12] Gibbons J, Holm D D and Kupershmidt B A 1983 The Hamiltonian structure of classical chromohydrodynamics *Phys.* D **6** 179–94
[13] Gibbons J, Holm D D and Tronci C 2008 Singular solutions for geodesic flows of Vlasov momentum moments *Probability, Geometry and Integrable Systems (Math. Sci. Res. Inst. Publ.* vol 55*)* ed M Pinsky and B Birnir (Cambridge: Cambridge University Press) pp 199–220
[14] Gibbons J, Holm D D and Tronci C 2008 Vlasov moments, integrable systems and singular solutions *Phys. Lett.* A **372** 1024–33
[15] Gilbert T L 2004 A phenomenological theory of damping in ferromagnetic materials *IEEE Trans. Magn.* **40** 3443–9
[16] Grmela M 1984 Bracket formulation of dissipative fluid mechanics equations *Phys. Lett.* A **102** 355–8
[17] Grmela M 1993 Weakly non-local hydrodynamics *Phys. Rev.* E **47** 351–65
[18] Grmela M 1993 Thermodynamics of driven systems *Phys. Rev.* E **48** 919–30
[19] Holm D D and Kupershmidt B 1988 The analogy between spin-glasses and Yang–Mills fluids *J. Math Phys.* **29** 21–30
[20] Holm D D, Marsden J E, Ratiu T S and Weinstein A 1985 Nonlinear stability of fluid and plasma equilibria *Phys. Rep.* **123** 1–116
[21] Holm D D and Putkaradze V 2005 Aggregation of finite-size particles with variable mobility *Phys. Rev. Lett.* **95** 226106
[22] Holm D D and Putkaradze V 2006 Formation of clumps and patches in self-aggregation of finite size particles *Physica* D **220** 183–96
[23] Holm D D and Putkaradze V 2007 Formation and evolution of singularities in anisotropic geometric continua *Physica* D **235** 33–47
[24] Holm D D, Putkaradze V and Stechmann S 2004 Rotating concentric circular peakons *Nonlinearity* **17** 2163–86
[25] Holm D D, Putkaradze V and Tronci C 2007 Double bracket dissipation in kinetic theory for particles with anisotropic interactions *Proc. Summer School and Conf. on Poisson Geometry (Trieste, Italy, 4-22 July, 2005)* (*Preprint* 0707.4204)
[26] Holm D D, Putkaradze V and Tronci C 2007 Geometric dissipation in kinetic equations *C. R. Acad. Sci., Paris* **345** 297–302
[27] Hoskins B J, McIntyre M E and Robertson A W 1985 On the use and significance of isentropic potential vorticity maps *Quart. J. Roy. Met. Soc.* **111** 877–946
[28] Kandrup H E 1990 Geometric approach to secular and nonlinear stability for spherical star clusters *Astrophy. J.* **351** 104–13
[29] Kandrup H E 1991 The secular instability of axisymmetric collisionless star cluster *Astrophys. J.* **380** 511–4
[30] Kaufman A N 1984 Dissipative Hamiltonian systems: a unifying principle *Phys. Lett.* A **100** 419–22
[31] Kraichnan R H 1967 Inertial ranges in two-dimensional turbulence *Phys. Fluids* **10** 1417–23
[32] Kupershmidt B A 1987 Hydrodynamical Poisson brackets and local Lie algebras *Phys. Lett.* A **121** 167–74
[33] Landau L D and Lifshitz E M 1935 On the theory of the dispersion of magnetic permeability in ferromagnetic bodies *Phys. Z. Sowjet.* **8** 153–69
see also Landau L D 1967 *Collected Papers* ed D Ter Haar (New York: Gordon and Breach)
[34] Matthaeus W H and Montgomery D 1980 Selective decay hypothesis at high mechanical and magnetic Reynolds numbers *Ann. New York Acad. Sci.* **357** 203–22
[35] Morrison P J 1984 Bracket formulation for irreversible classical fields *Phys. Lett.* A **100** 423–7
[36] Moser J and Veselov A 1991 Discrete version of some classical integrable systems and factorization of matrix polynomials *Commun. Math. Phys.* **139** 217–43
[37] Öttinger H C 2005 *Beyond Equilibrium Thermodynamics* (New York: Wiley)
[38] Otto F 2001 The geometry of dissipative evolution equations: the porous medium equation *Commun. Partial Differential Equations* **26** 101–74
[39] Paramonov L and Yaliraki S N 2005 The directional contact distance of two ellipsoids: coarse-grained potentials for anisotropic interactions *J. Chem. Phys.* **123** 194111
[40] Simo J C, Marsden J E and Krishnaprasad P S 1988 The Hamiltonian structure of nonlinear elasticity: the material and convective representations of solids, rods and plates *Arch. Ration. Mech. Anal.* **104** 125–83

[41] Sun S, Murray C B, Weller D, Folks L and Moser A 2000 Monodisperse FePt nano-particles and ferromagnetic FePt nano-crystal superlattices *Science* **287** 1989–92
[42] Taylor J B 1986 Relaxation and magnetic reconnection in plasmas *Rev. Mod. Phys.* **58** 741–63
[43] Tuberkevich V and Slavin A 2007 Nonlinear phenomenological model of magnetic dissipation for large precession angles: generalization of the Gilbert model *Phys. Rev.* B **75** 014440
[44] Vallis G K, Carnevale G F and Young W R 1989 Extremal energy properties and construction of stable solutions of the Euler equations *J. Fluid Mech.* **207** 133–52
[45] Young W R Selective decay of enstrophy and the excitation of barotropic waves in a channel *J. Atmos. Sci.* **44** 2804–12
[46] Zeng H, Li J, Liu J P, Wang Z L and Sun S 2002 Exchange-coupled nanocomposite magnets by nano-particle self-assembly *Nature* **420** 395–8