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Lagrangian analysis of alignment dynamics for isentropic compressible magnetohydrodynamics

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Abstract. After a review of the isentropic compressible magnetohydrodynamics (ICMHD) equations, a quaternionic framework for studying the alignment dynamics of a general fluid flow is explained and applied to the ICMHD equations.

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1. Introduction to isentropic compressible magnetohydrodynamics (ICMHD)

Consistent with the topic of this focus issue, this paper will deal with the equations of ICMHD [1]–[3]. Not only are these sufficiently general to encompass most of the interest in this area but they also offer a significant challenge even without dissipation. The ICMHD equations determine the dynamics of a conducting fluid flow with magnetic field $\boldsymbol{B}$ satisfying $\operatorname{div}\boldsymbol{B}=0$ and current $\boldsymbol{J}=\operatorname{curl}\boldsymbol{B}$. The equations for the fluid velocity field $\boldsymbol{u}$, mass density ρ, specific entropy σ, pressure $p(\rho,\sigma)$ and divergenceless magnetic field $\boldsymbol{B}$ are, respectively, the motion equation, Faraday's law of frozen-in magnetic flux, isentropy along flow lines and the continuity equation

$$\rho\frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t}=-\nabla p+\boldsymbol{J}\times\boldsymbol{B},\quad \frac{\partial\boldsymbol{B}}{\partial t}=\operatorname{curl}(\boldsymbol{u}\times\boldsymbol{B}),\tag{1.1}$$

$$\frac{\mathrm{D}\sigma}{\mathrm{D}t}=0,\quad \frac{\mathrm{D}\rho^{-1}}{\mathrm{D}t}=\rho^{-1}\operatorname{div}\boldsymbol{u},\tag{1.2}$$

with the Lagrangian time derivative defined as

$$\frac{\mathrm{D}}{\mathrm{D}t}=\frac{\partial}{\partial t}+\boldsymbol{u}\cdot\nabla.\tag{1.3}$$

The equation of state for specific internal energy $e(\rho,\sigma)$ and the thermodynamic first law yield

$$\frac{\mathrm{D}e}{\mathrm{D}t}=-p\frac{\mathrm{D}\rho^{-1}}{\mathrm{D}t}+T\frac{\mathrm{D}\sigma}{\mathrm{D}t}=-\frac{p}{\rho}\operatorname{div}\boldsymbol{u},\tag{1.4}$$

so the specific internal energy changes only because of mechanical work. Combining Faraday's law with the continuity equation yields

$$\frac{\mathrm{D}\boldsymbol{B}_\rho}{\mathrm{D}t}-\boldsymbol{B}_\rho\cdot\nabla\boldsymbol{u}=0\quad\text{with}\quad \boldsymbol{B}_\rho:=\rho^{-1}\boldsymbol{B}.\tag{1.5}$$

This is the condition for the vector field $\boldsymbol{B}_\rho\cdot\nabla$ to be frozen into the flow, i.e.

$$\frac{\mathrm{D}}{\mathrm{D}t}\left(\boldsymbol{B}_\rho\cdot\frac{\partial}{\partial\boldsymbol{x}}\right)=0,\quad\text{along}\quad \frac{\mathrm{D}\boldsymbol{x}}{\mathrm{D}t}:=\boldsymbol{u}.\tag{1.6}$$

We denote

$$\varpi:=p+\tfrac{1}{2}B^2,\tag{1.7}$$

and set

$$\frac{\mathrm{d}}{\mathrm{d}s}:=\boldsymbol{B}_\rho\cdot\nabla,\tag{1.8}$$

with $\boldsymbol{B}_\rho$ defined in (1.5). In this notation, the ICMHD equations (1.1) and (1.2) transform using standard vector identities into

$$\frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t} = \frac{\mathrm{d}\boldsymbol{B}}{\mathrm{d}s} - \rho^{-1}\nabla\varpi =: \boldsymbol{F}, \quad \frac{\mathrm{D}\boldsymbol{B}_\rho}{\mathrm{D}t} = \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}s}, \tag{1.9}$$

$$\frac{\mathrm{D}\sigma}{\mathrm{D}t} = 0 \quad \frac{\mathrm{D}\rho^{-1}}{\mathrm{D}t} = \rho^{-1}\mathrm{div}\,\boldsymbol{u}. \tag{1.10}$$

$\mathrm{D}/\mathrm{D}t$ and $\mathrm{d}/\mathrm{d}s$ are defined in (1.3) and (1.8) respectively. The first equation in (1.9) expresses the motion equation in terms of the derivative along field lines, while the second expresses Faraday's law (1.5) in terms of the derivatives $\mathrm{D}/\mathrm{D}t$ and $\mathrm{d}/\mathrm{d}s$. The invariance condition (1.6) for vector field $\mathrm{d}/\mathrm{d}s = \boldsymbol{B}_\rho \cdot \nabla$ along Lagrangian field lines for ICMHD implies equality of the following cross derivatives

$$\frac{\mathrm{D}}{\mathrm{D}t}\frac{\mathrm{d}}{\mathrm{d}s} = \frac{\mathrm{d}}{\mathrm{d}s}\frac{\mathrm{D}}{\mathrm{D}t}. \tag{1.11}$$

Of course, the invariant vector field $\mathrm{d}/\mathrm{d}s = \boldsymbol{B}_\rho \cdot \nabla$ may be applied to any fluid quantity. For example, applying $\mathrm{d}/\mathrm{d}s$ to the equations in (1.9) and using the equality of cross derivatives in $\mathrm{d}/\mathrm{d}s$ and $\mathrm{D}/\mathrm{D}t$ yields the following exact nonlinear wave equations for ICMHD

$$\frac{\mathrm{D}^2(\rho^{-1}\boldsymbol{B})}{\mathrm{D}t^2} - \frac{\mathrm{d}^2\boldsymbol{B}}{\mathrm{d}s^2} = -\frac{\mathrm{d}}{\mathrm{d}s}\left(\rho^{-1}\nabla\varpi\right), \tag{1.12}$$

$$\frac{\mathrm{D}^2\boldsymbol{u}}{\mathrm{D}t^2} - \frac{\mathrm{d}^2\boldsymbol{u}}{\mathrm{d}s^2} = -\frac{\mathrm{D}}{\mathrm{D}t}\left(\rho^{-1}\nabla\varpi\right). \tag{1.13}$$

When linearized, these equations yield Alfvén-sound waves. The present work emphasizes the alignment dynamics that is inherent in these equations, rather than their wave properties.

1.1. Slow plus fast decomposition and nonlinear waves

It seems natural to define slow and fast aspects of the ICMHD solutions in the sense of the Lagrangian time derivative. In particular, there are two relations for slow variables

$$\frac{\mathrm{D}\sigma}{\mathrm{D}t} = 0, \quad \text{and} \quad \frac{\mathrm{D}\beta}{\mathrm{D}t} = 0, \tag{1.14}$$

where β is defined as

$$\beta := \boldsymbol{B}_\rho \cdot \nabla\sigma. \tag{1.15}$$

The latter follows from equality of cross derivatives, by computing

$$\frac{\mathrm{D}\beta}{\mathrm{D}t} := \frac{\mathrm{D}}{\mathrm{D}t}(\boldsymbol{B}_\rho \cdot \nabla\sigma) = \frac{\mathrm{D}}{\mathrm{D}t}\frac{\mathrm{d}\sigma}{\mathrm{d}s} = \frac{\mathrm{d}}{\mathrm{d}s}\frac{\mathrm{D}\sigma}{\mathrm{D}t} = 0. \tag{1.16}$$

Thus, the ICMHD equations preserve the projection of $\boldsymbol{B}_\rho$ on $\nabla\sigma$ along *Lagrangian flow lines*, that is, along the path $\boldsymbol{x}(t)$ of a Lagrangian fluid particle determined from $\mathrm{d}\boldsymbol{x}/\mathrm{d}t = \boldsymbol{u}(\boldsymbol{x}, t)$.

Equivalently, one finds the Eulerian conservation law,

$$\frac{\partial(\rho\beta)}{\partial t} + \mathrm{div}(\rho\beta\boldsymbol{u}) = 0, \quad \text{with} \quad \rho\beta = \boldsymbol{B}\cdot\nabla\sigma = \mathrm{div}(\sigma\boldsymbol{B}), \tag{1.17}$$

upon combining (1.16) with the continuity equation for mass.

Of course, the evolution of the component of $\boldsymbol{B}_\rho$ *perpendicular* to $\nabla\sigma$ is not so simple! One may decompose $\boldsymbol{B}_\rho$ into components parallel and perpendicular to $\nabla\sigma$ as

$$|\nabla\sigma|^2\boldsymbol{B}_\rho = \beta\nabla\sigma + \boldsymbol{\gamma}\times\nabla\sigma = |\nabla\sigma|^2(\boldsymbol{B}_\rho^{\parallel} + \boldsymbol{B}_\rho^{\perp}) \quad \text{with} \quad \boldsymbol{\gamma}\cdot\nabla\sigma = 0, \tag{1.18}$$

so that

$$\beta = \boldsymbol{B}_\rho\cdot\nabla\sigma \quad \text{and} \quad \boldsymbol{\gamma} = \boldsymbol{B}_\rho\times\nabla\sigma. \tag{1.19}$$

One then computes the auxiliary equations,

$$\frac{\mathrm{D}}{\mathrm{D}t}\nabla\sigma = -(\nabla\boldsymbol{u})^{\mathrm{T}}\cdot\nabla\sigma\,, \qquad \text{that is,} \qquad \frac{\mathrm{D}\sigma_{,i}}{\mathrm{D}t} = -\sigma_{,j}u^j_{,i}, \tag{1.20}$$

and

$$\frac{\mathrm{D}}{\mathrm{D}t}|\nabla\sigma|^2 = -\nabla\sigma\cdot S\cdot\nabla\sigma. \tag{1.21}$$

The fluid strain-rate tensor is defined as $S = \frac{1}{2}(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^{\mathrm{T}})$. Consequently, the evolution equation for the component of $\boldsymbol{B}_\rho$ *perpendicular* to $\nabla\sigma$ is determined from

$$\frac{\mathrm{D}\boldsymbol{\gamma}}{Dt} = \frac{\mathrm{D}}{\mathrm{D}t}(\boldsymbol{B}_\rho\times\nabla\sigma) = \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}s}\times\nabla\sigma - \boldsymbol{B}_\rho\times(\nabla\boldsymbol{u}^{\mathrm{T}}\cdot\nabla\sigma) \tag{1.22}$$

which is clearly neither fast nor slow.

1.2. Lagrangian dynamics of specific volume

Two other likely candidates for fast variables are the specific volume ρ^{-1} and the velocity divergence $\mathrm{div}\,\boldsymbol{u}$, which satisfy

$$\frac{\mathrm{D}\rho^{-1}}{\mathrm{D}t} = \rho^{-1}\mathrm{div}\,\boldsymbol{u}, \tag{1.23}$$

$$\frac{\mathrm{D}}{\mathrm{D}t}\mathrm{div}\,\boldsymbol{u} = \mathrm{div}\,\boldsymbol{F} - |\nabla\boldsymbol{u}|^2. \tag{1.24}$$

The second of these equations is found using the identity

$$\frac{\mathrm{D}}{\mathrm{D}t}\mathrm{div}\,\boldsymbol{u} = \mathrm{div}\left(\frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t}\right) - |\nabla\boldsymbol{u}|^2 \tag{1.25}$$

where $|\nabla \boldsymbol{u}|^2 \equiv u^i_{\,,j} u^j_{\,,i}$. As a consequence of (1.23) and (1.24), the specific volume ρ^{-1} satisfies the 'Lagrangian oscillation equation,'

$$\frac{\mathrm{D}^2 \rho^{-1}}{\mathrm{D}t^2} = \rho^{-1}\left((\mathrm{div}\boldsymbol{u})^2 - |\nabla \boldsymbol{u}|^2 + \mathrm{div}\left(\frac{\mathrm{d}\boldsymbol{B}}{\mathrm{d}s} - \rho^{-1}\nabla\varpi \right)\right) \tag{1.26}$$

upon substituting the definition of force $\boldsymbol{F} := \frac{\mathrm{d}\boldsymbol{B}}{\mathrm{d}s} - \rho^{-1}\nabla\varpi$. Thus, the divergence of the force combines with compressibility of the flow to drive either Lagrangian oscillations or exponential variations of the specific volume, depending on the sign of the term on the right-hand side of equation (1.26). Of course, the sign of this term could be varying rapidly in some physical applications, and observations of such behaviour would have corresponding implications for the dynamics of specific volume. In any case, the form of equation (1.26) is universal and one may conclude that the divergence of the total force drives the second Lagrangian time derivative of the specific volume.

In what follows, we shall seek equations for alignment dynamics in MHD which have the same universal property as the Lagrangian oscillation equation (1.26). In particular, we shall find that *gradients* of the total force (rather than its divergence) drive the Lagrangian dynamics of alignment in MHD of the frozen-in magnetic vector field $\boldsymbol{B}_\rho$ relative to its projection $\boldsymbol{B}_\rho \cdot \nabla \boldsymbol{u}$ on to the shear tensor $\nabla \boldsymbol{u}$ of the fluid velocity.

1.3. Stretching and alignment

The magnetic flux equation

$$\frac{\mathrm{D}\boldsymbol{B}_\rho}{\mathrm{D}t} = \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}s} := \boldsymbol{B}_\rho \cdot \nabla \boldsymbol{u} \tag{1.27}$$

implies that the contravariant vector $\boldsymbol{B}_\rho$ undergoes stretching to the extent it aligns with the shear $\nabla \boldsymbol{u}$. Likewise, this alignment evolves according to

$$\frac{\mathrm{D}^2\boldsymbol{B}_\rho}{\mathrm{D}t^2} = \frac{\mathrm{D}}{\mathrm{D}t}\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}s} = \frac{\mathrm{d}}{\mathrm{d}s}\frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t} = \frac{\mathrm{d}}{\mathrm{d}s}\boldsymbol{F} = \frac{\mathrm{d}}{\mathrm{d}s}\left(\frac{\mathrm{d}\boldsymbol{B}}{\mathrm{d}s} - \rho^{-1}\nabla\varpi \right), \tag{1.28}$$

which recovers the nonlinear wave equation (1.12) above.

We shall examine this equation from an alignment viewpoint, rather than as a wave propagation phenomenon. We begin by decomposing the vector $\boldsymbol{B}_\rho \cdot \nabla \boldsymbol{u}$ into its components parallel and perpendicular to $\hat{\boldsymbol{B}}_\rho := \boldsymbol{B}_\rho / |\boldsymbol{B}_\rho|$

$$\boldsymbol{B}_\rho \cdot \nabla \boldsymbol{u} = \alpha\, \hat{\boldsymbol{B}}_\rho + \boldsymbol{\chi} \times \hat{\boldsymbol{B}}_\rho\,, \tag{1.29}$$

where α and $\boldsymbol{\chi}$ are defined by

$$\alpha = \hat{\boldsymbol{B}}_\rho \cdot (\hat{\boldsymbol{B}}_\rho \cdot \nabla \boldsymbol{u}), \quad \text{and} \quad \boldsymbol{\chi} = \hat{\boldsymbol{B}}_\rho \times (\hat{\boldsymbol{B}}_\rho \cdot \nabla \boldsymbol{u}). \tag{1.30}$$

This decomposition is explained more fully in section 2.2. In fact, α is the Lagrangian amplification rate of the magnitude $|\boldsymbol{B}_\rho|$ and $\boldsymbol{\chi}$ is the Lagrangian frequency of rotation of the unit vector $\hat{\boldsymbol{B}}_\rho$ under the forcing by shear in the flux conservation equation (1.27),

$$\frac{\mathrm{D}|\boldsymbol{B}_\rho|}{\mathrm{D}t} = \alpha\, |\boldsymbol{B}_\rho| \quad \text{and} \quad \frac{\mathrm{D}\hat{\boldsymbol{B}}_\rho}{\mathrm{D}t} = \boldsymbol{\chi} \times \hat{\boldsymbol{B}}_\rho. \tag{1.31}$$

Note that no confusion should arise between this α and the one appearing in the α-dynamo equations!

1.4. A mathematical framework for magnetic fluid alignment dynamics

The quantity α defined in equation (1.30) is the *alignment* of $\boldsymbol{B}_\rho$ with $\nabla\boldsymbol{u}$, which determines the rates of change of magnitude $|\boldsymbol{B}_\rho|$ whereas $\boldsymbol{\chi}$ is the *misalignment*, which determines the frequency of rotation of the direction $\hat{\boldsymbol{B}}_\rho$. The question asked in this situation is, 'How long will $\boldsymbol{B}_\rho$ remain aligned with $\nabla\boldsymbol{u}$, so it can continue to be stretched under the fluid shear?' Answering this question requires an analysis of $\mathrm{D}\alpha/\mathrm{D}t$ and $\mathrm{D}\boldsymbol{\chi}/\mathrm{D}t$ using the alignment dynamics (1.28).

In principle, this analysis could be performed by direct computation and algebraic manipulation. However, the Lagrangian evolution equations for α and $\boldsymbol{\chi}$ happen to fit perfectly into a mathematical framework that was especially designed for analysing orientation dynamics and for systematically interpreting the results. The key for recognizing this framework is to notice that the decomposition of a vector into its components parallel and perpendicular to another vector defines a type of product, or multiplication, that was first discovered by Hamilton [4]. This product reveals itself when we write the parallel-perpendicular vector decomposition equation (1.29) as though it were the pure vector components of a equation involving the four-component scalar-vector object (tetrad) $[\alpha,\ \boldsymbol{\chi}]$ in the form,

$$[0,\, \boldsymbol{B}_\rho \cdot \nabla\boldsymbol{u}] = [0,\, \alpha\,\hat{\boldsymbol{B}}_\rho + \boldsymbol{\chi} \times \hat{\boldsymbol{B}}_\rho] = [\alpha,\, \boldsymbol{\chi}] \circledast [0,\, \hat{\boldsymbol{B}}_\rho] \quad \text{with} \quad \boldsymbol{\chi} \cdot \hat{\boldsymbol{B}}_\rho = 0. \tag{1.32}$$

This organization of the decomposition equation (1.29) summons the $\circledast$ product defined by

$$[p_1, \boldsymbol{q}_1] \circledast [p_2, \boldsymbol{q}_2] = [p_1 p_2 - \boldsymbol{q}_1 \cdot \boldsymbol{q}_2,\, p_1\boldsymbol{q}_2 + \boldsymbol{q}_1 p_2 + \boldsymbol{q}_1 \times \boldsymbol{q}_2], \tag{1.33}$$

which is the multiplication rule that Hamilton invented for the field of quaternions [4]. The origin of this rule and its connection to the definition of a quaternion is given in section 2.1. Of course, quaternions have everything to do with orientation [5, 6]. The remainder of this paper sets-up the quaternionic framework for alignment dynamics of a general fluid flow and applies it to the ICMHD equations.

The plan of this paper is as follows: section 2 summarizes the results of [7, 8] and shows how the evolution of the ortho-normal frame can be calculated in general terms. Section 3 then discusses the ICMHD equations (1.9) and (1.10) in these terms, while section 4 examines alignment and growth properties to begin answering the question raised above for magnetic dynamos using these results. Finally, section 5 discusses the potential for other applications of this general method in compressible MHD turbulence.

2. Quaternions and Lagrangian alignment dynamics

2.1. Background for quaternions

The resurgence of practical interest in quaternions during the last two decades has been stimulated by progress in the computer animation and inertial navigation industries because of the ease with which quaternions handle moving objects undergoing three-axis rotations [5, 6]. The tracking of aircraft and satellites and the animation of tumbling objects in computer graphics are obvious examples. Quaternion methods have also been recently been applied to the three-dimensional Euler equations for incompressible fluid motion [9, 10] and to passive tracer particles transported by an underlying Lagrangian flow field; see [11]–[21] and references in [7, 8]. The final result of these endeavours is that equations of motion can be derived for an ortho-normal frame. This 'quaternion frame' follows the evolution of particles in a Lagrangian flow whose evolution derives from the Eulerian equations of motion.

Three-axis rotations lie at the heart of the definition of a quaternion [22]. In terms of any scalar p and any three vector $\boldsymbol{q}$, the quaternion $\mathfrak{q} = [p,\ \boldsymbol{q}]$ is defined (using gothic fonts to denote quaternions) as

$$\mathfrak{q} = [p, \boldsymbol{q}] = pI - \sum_{i=1}^{3} q_i \sigma_i, \tag{2.1}$$

where $\{\sigma_1,\ \sigma_2,\ \sigma_3\}$ are the Pauli spin-matrices and I is the unit matrix. The relations between the Pauli matrices $\sigma_i \sigma_j = -\delta_{ij} I - \epsilon_{ijk} \sigma_k$ then give a non-commutative multiplication rule

$$\mathfrak{q}_1 \circledast \mathfrak{q}_2 = [p_1 p_2 - \boldsymbol{q}_1 \cdot \boldsymbol{q}_2,\ p_1 \boldsymbol{q}_2 + \boldsymbol{q}_1 p_2 + \boldsymbol{q}_1 \times \boldsymbol{q}_2]. \tag{2.2}$$

It is easily demonstrated that quaternions are associative. In fact the individual elements of a unit quaternion provide the Cayley–Klein parameters of a rotation. This representation is a standard alternative to Euler angles in describing the orientation of rotating objects, as the books by Whittaker and Klein show [23, 24].

2.2. *Quaternions and Lagrangian alignment dynamics in fluids*

A general quaternionic picture of the process of Lagrangian flow and acceleration in fluid dynamics is explained in this section by considering the abstract Lagrangian flow equation

$$\frac{\mathrm{D}\boldsymbol{w}}{\mathrm{D}t} = \boldsymbol{a}(\boldsymbol{x}, t), \tag{2.3}$$

whose Lagrangian acceleration equation is given in general by

$$\frac{\mathrm{D}^2\boldsymbol{w}}{\mathrm{D}t^2} = \frac{\mathrm{D}\boldsymbol{a}}{\mathrm{D}t} = \boldsymbol{b}(\boldsymbol{x}, t). \tag{2.4}$$

These are the rates of change of these vectors following the characteristics of the velocity generating the path $\boldsymbol{x}(t)$ of a Lagrangian fluid particle determined from $\mathrm{d}\boldsymbol{x}/\mathrm{d}t = \boldsymbol{u}(\boldsymbol{x},\ t)$.

Given the Lagrangian equation (2.3) one defines the scalar α_a and the three vector $\boldsymbol{\chi}_a$ as

$$\alpha_a = w^{-1}(\hat{\boldsymbol{w}} \cdot \boldsymbol{a}) \qquad \boldsymbol{\chi}_a = w^{-1}(\hat{\boldsymbol{w}} \times \boldsymbol{a}), \tag{2.5}$$

in which $\boldsymbol{w} = w\hat{\boldsymbol{w}}$ with $w = |\boldsymbol{w}|$. As observed in (1.29), the three vector $\boldsymbol{a}$ is decomposed into parts that are parallel and perpendicular to $\boldsymbol{w}$ as

$$\boldsymbol{a} = \alpha_a \boldsymbol{w} + \boldsymbol{\chi}_a \times \boldsymbol{w} = [\alpha_a,\ \boldsymbol{\chi}_a] \circledast [0,\ \boldsymbol{w}], \tag{2.6}$$

and thus the quaternionic product (2.6) is summoned in a natural manner. By definition, the growth rate α_a of the scalar magnitude $w = |\boldsymbol{w}|$ obeys

$$\frac{\mathrm{D}w}{\mathrm{D}t} = \alpha_a w, \tag{2.7}$$

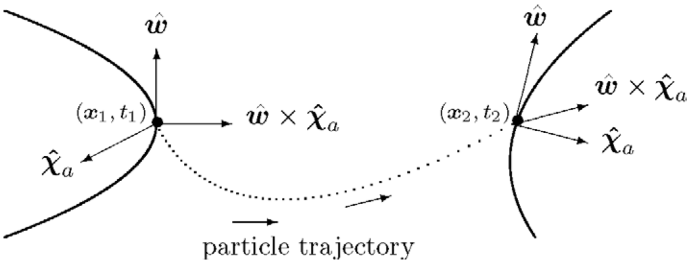

Figure 1. The dotted line represents the path of Lagrangian fluid particle (•) moving from $(\boldsymbol{x}_1, t_1)$ to $(\boldsymbol{x}_2, t_2)$. The solid curves represent lines of constant $\boldsymbol{w}$ to which $\hat{\boldsymbol{w}}$ is a unit tangent vector. The orientation of the quaternion-frame $(\hat{\boldsymbol{w}}, \hat{\boldsymbol{\chi}}_a, \hat{\boldsymbol{w}} \times \hat{\boldsymbol{\chi}}_a)$ is shown at the two space-time points; note that this is not the Frenet-frame corresponding to the particle path but to lines of constant $\boldsymbol{w}$.

while the unit tangent vector $\hat{\boldsymbol{w}} = \boldsymbol{w}w^{-1}$ satisfies

$$\frac{\mathrm{D}\hat{\boldsymbol{w}}}{\mathrm{D}t} = \boldsymbol{\chi}_a \times \hat{\boldsymbol{w}}. \tag{2.8}$$

Now define two quaternions

$$\mathfrak{q}_a = [\alpha_a, \boldsymbol{\chi}_a] \quad \text{and} \quad \mathfrak{q}_b = [\alpha_b, \boldsymbol{\chi}_b], \tag{2.9}$$

where α_b, $\boldsymbol{\chi}_b$ are defined as in (2.5) for α_a, $\boldsymbol{\chi}_a$ with $\boldsymbol{a}$ replaced by $\boldsymbol{b}$. Let $\mathfrak{w} = [0,\ \boldsymbol{w}]$ be the pure quaternion satisfying the Lagrangian evolution equation (2.3) with $\mathfrak{q}_a$ defined in (2.9). Then (2.3) can automatically be re-written equivalently in the quaternion form

$$\frac{\mathrm{D}\mathfrak{w}}{\mathrm{D}t} = [0, \boldsymbol{a}] = [0, \alpha_a \boldsymbol{w} + \boldsymbol{\chi}_a \times \boldsymbol{w}] = \mathfrak{q}_a \circledast \mathfrak{w}. \tag{2.10}$$

Moreover, if $\boldsymbol{a}$ is Lagrangian-differentiable as in (2.4) then it is clear that a similar decomposition for $\boldsymbol{b}$ as that for $\boldsymbol{a}$ in (2.6) gives

$$\frac{\mathrm{D}^2\mathfrak{w}}{\mathrm{D}t^2} = [0, \boldsymbol{b}] = [0, \alpha_b \boldsymbol{w} + \boldsymbol{\chi}_b \times \boldsymbol{w}] = \mathfrak{q}_b \circledast \mathfrak{w}. \tag{2.11}$$

Using the associativity property, compatibility of (2.11) and (2.10) implies that

$$\left(\frac{\mathrm{D}\mathfrak{q}_a}{\mathrm{D}t} + \mathfrak{q}_a \circledast \mathfrak{q}_a - \mathfrak{q}_b\right) \circledast \mathfrak{w} = 0, \tag{2.12}$$

which establishes a *Riccati relation* between the quaternions $\mathfrak{q}_a$ and $\mathfrak{q}_b$

$$\frac{\mathrm{D}\mathfrak{q}_a}{\mathrm{D}t} + \mathfrak{q}_a \circledast \mathfrak{q}_a = \mathfrak{q}_b. \tag{2.13}$$

From equation (2.13) there follows the main result of the paper.

Theorem 1. *(The ortho-normal quaternion-frame)* $F = (\hat{\boldsymbol{w}},\ \hat{\boldsymbol{\chi}}_a,\ \hat{\boldsymbol{w}} \times \hat{\boldsymbol{\chi}}_a) \in SO(3)$ *has Lagrangian time derivatives expressed as*

$$\frac{\mathrm{D}\hat{\boldsymbol{w}}}{\mathrm{D}t} = \boldsymbol{\mathcal{D}}_a \times \hat{\boldsymbol{w}}, \tag{2.14}$$

$$\frac{\mathrm{D}(\hat{\boldsymbol{w}} \times \hat{\boldsymbol{\chi}}_a)}{\mathrm{D}t} = \boldsymbol{\mathcal{D}}_a \times (\hat{\boldsymbol{w}} \times \hat{\boldsymbol{\chi}}_a), \tag{2.15}$$

$$\frac{\mathrm{D}\hat{\boldsymbol{\chi}}_a}{\mathrm{D}t} = \boldsymbol{\mathcal{D}}_a \times \hat{\boldsymbol{\chi}}_a, \tag{2.16}$$

where the Darboux vector $\boldsymbol{\mathcal{D}}_a$ *defined as*

$$\boldsymbol{\mathcal{D}}_a = \frac{c_b}{\chi_a}\hat{\boldsymbol{w}} + \boldsymbol{\chi}_a \quad \text{with} \quad c_b = \boldsymbol{\chi}_b \cdot (\hat{\boldsymbol{w}} \times \hat{\boldsymbol{\chi}}_a), \tag{2.17}$$

is the angular frequency of rotation of the ortho-normal frame F.

Remark.

1. The frame orientation is controlled by the Darboux vector $\boldsymbol{\mathcal{D}}_a = (c_b/\chi_a,\ 0,\ \chi_a)$ which lies in the $(\hat{\boldsymbol{w}},\ \hat{\boldsymbol{\chi}}_a)$ plane and is so named for its similarity to the Darboux vector in the Frenet–Serret (FS) equations for a space curve. Note that the vector $\boldsymbol{\mathcal{D}}_a$ depends on $\boldsymbol{\chi}_b$ but is independent of α_b.
2. The frame dynamics equations (2.14)–(2.17) may also be re-written in matrix form by defining the 3×3 skew-symmetric matrix $C_a \in so(3)$ with entries $[C_a]_{ij} = -\epsilon_{ijk}D_a^k$ as,

$$\frac{\mathrm{D}F}{\mathrm{D}t} = C_a F \quad \text{where} \quad F = \begin{pmatrix} \hat{\boldsymbol{w}} \\ \hat{\boldsymbol{w}} \times \boldsymbol{\chi}_a \\ \boldsymbol{\chi}_a \end{pmatrix} \quad \text{and} \quad C_a = \begin{pmatrix} 0 & -\chi_a & 0 \\ \chi_a & 0 & -c_b/\chi_a \\ 0 & c_b/\chi_a & 0 \end{pmatrix}. \tag{2.18}$$

Proof. Finding an expression for the Lagrangian time derivatives of the components of the frame $(\hat{\boldsymbol{w}},\ \hat{\boldsymbol{w}} \times \hat{\boldsymbol{\chi}}_a,\ \hat{\boldsymbol{\chi}}_a)^{\mathrm{T}}$ requires the derivative of $\hat{\boldsymbol{\chi}}_a$. For this, one first recalls that the three vector $\boldsymbol{b}$ may be expressed in this ortho-normal frame as the linear combination

$$w^{-1}\boldsymbol{b} = \alpha_b\hat{\boldsymbol{w}} + c_b\hat{\boldsymbol{\chi}}_a + d_b(\hat{\boldsymbol{w}} \times \hat{\boldsymbol{\chi}}_a), \tag{2.19}$$

where c_b is defined in (2.17) and $d_b = -(\hat{\boldsymbol{\chi}}_a \cdot \boldsymbol{\chi}_b)$. The three vector product $\boldsymbol{\chi}_b = w^{-1}(\hat{\boldsymbol{w}} \times \boldsymbol{b})$ yields

$$\hat{\boldsymbol{\chi}}_b = c_b(\hat{\boldsymbol{w}} \times \hat{\boldsymbol{\chi}}_a) - d_b\hat{\boldsymbol{\chi}}_a. \tag{2.20}$$

To find the Lagrangian time derivative of $\hat{\boldsymbol{\chi}}_a$, we use the three vector part of the equation for the quaternion $\mathfrak{q}_a = [\alpha_a,\ \boldsymbol{\chi}_a]$ in theorem 1

$$\frac{\mathrm{D}\boldsymbol{\chi}_a}{\mathrm{D}t} = -2\alpha_a\boldsymbol{\chi}_a + \boldsymbol{\chi}_b, \qquad \Rightarrow \qquad \frac{\mathrm{D}\chi_a}{\mathrm{D}t} = -2\alpha_a\chi_a - d_b, \tag{2.21}$$

where $\chi_a = |\boldsymbol{\chi}_a|$. Using (2.20) and (2.21) there follows

$$\frac{\mathrm{D}\hat{\boldsymbol{\chi}}_a}{\mathrm{D}t} = c_b\chi_a^{-1}(\hat{\boldsymbol{w}} \times \hat{\boldsymbol{\chi}}_a), \qquad \frac{\mathrm{D}(\hat{\boldsymbol{w}} \times \hat{\boldsymbol{\chi}}_a)}{\mathrm{D}t} = \chi_a\hat{\boldsymbol{w}} - c_b\chi_a^{-1}\hat{\boldsymbol{\chi}}_a, \tag{2.22}$$

which gives equations (2.14)–(2.17). □

3. Application of the quaternionic alignment theorem to ICMHD

The way is now clear to apply theorem 1 of section 2 to the ICMHD equations (1.9) and (1.10). First, we identify from (1.27) and (1.28)

$$\boldsymbol{w} = \boldsymbol{B}_\rho, \quad \boldsymbol{a} = \boldsymbol{B}_\rho \cdot \nabla \boldsymbol{u}, \quad \boldsymbol{b} = \frac{\mathrm{D}(\boldsymbol{B}_\rho \cdot \nabla \boldsymbol{u})}{\mathrm{D}t} = \boldsymbol{B}_\rho \cdot \nabla \left(\frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t}\right). \tag{3.1}$$

The latter result is achieved through the use of Ertl's theorem (see [10, 28, 29]). Although messy, this provides an explicit expression for $\boldsymbol{b}$ that depends upon the pressure p, $\boldsymbol{B}_\rho$, $\boldsymbol{J}$ and their derivatives, as determined from the fluid evolution equations for $\boldsymbol{u}$, ρ and σ,

$$\boldsymbol{b} = \boldsymbol{B}_\rho \cdot \nabla(-\rho^{-1}\nabla p + \boldsymbol{J} \times \boldsymbol{B}_\rho). \tag{3.2}$$

The alignment parameters $\{\alpha,\ \boldsymbol{\chi},\ \alpha_b,\ \boldsymbol{\chi}_b\}$ are now identified as

$$\alpha = \hat{\boldsymbol{B}}_\rho \cdot (\hat{\boldsymbol{B}}_\rho \cdot \nabla \boldsymbol{u}), \quad \boldsymbol{\chi} = \hat{\boldsymbol{B}}_\rho \times (\hat{\boldsymbol{B}}_\rho \cdot \nabla \boldsymbol{u}), \tag{3.3}$$

$$\alpha_b = |\boldsymbol{B}_\rho|^{-1}(\hat{\boldsymbol{B}}_\rho \cdot \boldsymbol{b}), \quad \boldsymbol{\chi}_b = |\boldsymbol{B}_\rho|^{-1}(\hat{\boldsymbol{B}}_\rho \times \boldsymbol{b}). \tag{3.4}$$

These parameters appear in the vector decompositions,

$$\boldsymbol{a} = \boldsymbol{B}_\rho \cdot \nabla \boldsymbol{u} = \alpha\, \hat{\boldsymbol{B}}_\rho + \boldsymbol{\chi} \times \hat{\boldsymbol{B}}_\rho\,, \tag{3.5}$$

and

$$\boldsymbol{b} = \boldsymbol{B}_\rho \cdot \nabla \left(\frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t}\right) = \alpha_b \hat{\boldsymbol{B}}_\rho + \boldsymbol{\chi}_b \times \hat{\boldsymbol{B}}_\rho\,. \tag{3.6}$$

The parameters α_b and $\boldsymbol{\chi}_b$ derive from $\boldsymbol{B}_\rho$ and from $\boldsymbol{b}$ in equation (3.2) at each time step. The vector $\boldsymbol{b}$ represents the coupling of the kinematic flow variables $(\boldsymbol{B}_\rho, \nabla \boldsymbol{u})$ to the *gradients* of the magnetic and thermodynamic forces. These identifications enter the two quaternions $\mathfrak{q} = [\alpha,\ \boldsymbol{\chi}]$ and $\mathfrak{q}_b = [\alpha_b,\ \boldsymbol{\chi}_b]$ that satisfy the Riccati equation (2.13). The results of theorem 1 for the Lagrangian time derivatives of the orthonormal frame $F_{\mathrm{mag}} = (\hat{\boldsymbol{B}}_\rho\,, \hat{\boldsymbol{B}}_\rho \times \hat{\boldsymbol{\chi}}\,, \hat{\boldsymbol{\chi}})^{\mathrm{T}} \in SO(3)$ are then expressed as

$$\frac{\mathrm{D}\hat{\boldsymbol{B}}_\rho}{\mathrm{D}t} = \boldsymbol{\mathcal{D}} \times \hat{\boldsymbol{B}}_\rho, \tag{3.7}$$

$$\frac{\mathrm{D}(\hat{\boldsymbol{B}}_\rho \times \hat{\boldsymbol{\chi}})}{\mathrm{D}t} = \boldsymbol{\mathcal{D}} \times (\hat{\boldsymbol{B}}_\rho \times \hat{\boldsymbol{\chi}}), \tag{3.8}$$

$$\frac{\mathrm{D}\hat{\boldsymbol{\chi}}}{\mathrm{D}t} = \boldsymbol{\mathcal{D}} \times \hat{\boldsymbol{\chi}}, \tag{3.9}$$

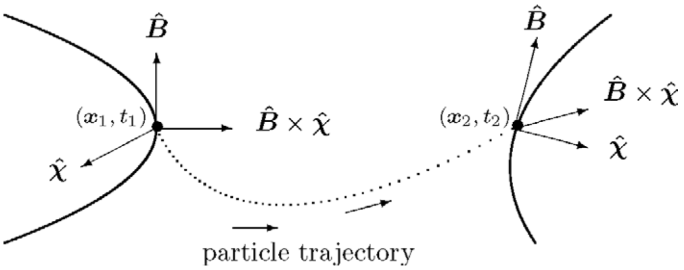

Figure 2. The solid curves represent magnetic field lines to which $\hat{\boldsymbol{B}}$ is a unit tangent vector. The dotted line represents the path of a Lagrangian fluid particle (•) moving from $(\boldsymbol{x}_1, t_1)$ to $(\boldsymbol{x}_2, t_2)$. The orientation of the quaternion-frame $(\hat{\boldsymbol{B}}, \hat{\boldsymbol{\chi}}, \hat{\boldsymbol{B}} \times \hat{\boldsymbol{\chi}})$ is shown at the two space-time points.

where the Darboux angular velocity vector $\boldsymbol{\mathcal{D}}$ is defined as

$$\boldsymbol{\mathcal{D}} = \frac{c_b}{\chi}\hat{\boldsymbol{B}}_\rho + \boldsymbol{\chi}, \quad \text{with} \quad c_b = \boldsymbol{\chi}_b \cdot (\hat{\boldsymbol{B}}_\rho \times \hat{\boldsymbol{\chi}}), \tag{3.10}$$

which depends explicitly on the ICMHD force gradients through $\boldsymbol{\chi}_b$ but is independent of α_b.

The frame dynamics equations (3.7)–(3.10) for ICMHD may also be re-written in matrix form using the 3×3 skew-symmetric matrix $C \in so(3)$ with entries $C_{ij} = -\epsilon_{ijk} D^k$ as,

$$\frac{\mathrm{D}F_{\mathrm{mag}}}{\mathrm{D}t} = CF_{\mathrm{mag}} \quad \text{where} \quad F_{\mathrm{mag}} = \begin{pmatrix} \hat{\boldsymbol{B}}_\rho \\ \hat{\boldsymbol{B}}_\rho \times \hat{\boldsymbol{\chi}} \\ \hat{\boldsymbol{\chi}} \end{pmatrix} \quad \text{and} \quad C = \begin{pmatrix} 0 & -\chi & 0 \\ \chi & 0 & -c_b/\chi \\ 0 & c_b/\chi & 0 \end{pmatrix}. \tag{3.11}$$

Remark.

1. The skew-symmetric matrix $C = \frac{\mathrm{D}F_{\mathrm{mag}}}{\mathrm{D}t} F_{\mathrm{mag}}^{-1}$ expresses the Lagrangian angular frequency of rotation of the magnetic orthonormal frame F_{mag} in terms of the magnitudes χ and c_b.
2. At a given moment in time, the flow lines of $\boldsymbol{B}_\rho$ may be constructed from its characteristic equations $\mathrm{d}\boldsymbol{x}/\mathrm{d}s = \boldsymbol{B}_\rho(\boldsymbol{x})$. The FS equations describe how the orientation of an orthonormal frame changes along each flow line of $\boldsymbol{B}_\rho$ as a function of its shape parameters, curvature and torsion. Applying equality of cross derivatives to equations (3.11) and FS yields a relation for the Lagrangian time derivatives of the shape parameters of a given flow line of $\boldsymbol{B}_\rho$.

Figure 1 now becomes figure 2.

4. Alignment and growth properties in ICMHD

The growth rate $\alpha(\boldsymbol{x}, t)$, defined in (3.3), satisfies (see equations (2.7) and (2.8))

$$\frac{\mathrm{D}|\boldsymbol{B}_\rho|}{\mathrm{D}t} = \alpha|\boldsymbol{B}_\rho|. \tag{4.1}$$

Here α can take either sign and this is the key to how fast the magnitude $|\boldsymbol{B}_\rho|$ increases (or decreases) at each point in the flow. In contrast, the three vector $\boldsymbol{\chi}(\boldsymbol{x}, t)$ is the key to the alignment properties of the system, because it satisfies

$$\frac{D\hat{\boldsymbol{B}}_\rho}{Dt} = \boldsymbol{\chi} \times \hat{\boldsymbol{B}}_\rho. \tag{4.2}$$

As such, it can be interpreted as the swing rate of the unit vector $\hat{\boldsymbol{B}}_\rho$ about $\boldsymbol{a} = \boldsymbol{B}_\rho \cdot \nabla \boldsymbol{u}$. Clearly, if $\boldsymbol{B}_\rho$ is aligned with $\boldsymbol{a}$ then $\boldsymbol{\chi} = 0$ and the quaternion $\mathfrak{q}$ involves only the scalar α. Violent corkscrew-like motions of the magnetic field lines would be consistent with significant values of $\boldsymbol{\chi}$ and such motions can therefore be regarded as a diagnostic for the misalignment of $\hat{\boldsymbol{B}}_\rho$ with $\boldsymbol{a}$. One of the messages of this paper is that putting α and $\boldsymbol{\chi}$ together as the quaternion $\mathfrak{q} = [\alpha, \ \boldsymbol{\chi}]$ is a natural way to approach this problem because the full quaternion $\mathfrak{q}$ with $\boldsymbol{\chi} \neq 0$ is summoned whenever vortex or magnetic field lines bend or tangle. The Darboux vector $\boldsymbol{\mathcal{D}}$ is the angular frequency of rotation of the orthonormal frame $F_{\text{mag}} = (\hat{\boldsymbol{B}}_\rho\,, \hat{\boldsymbol{B}}_\rho \times \hat{\boldsymbol{\chi}}\,, \hat{\boldsymbol{\chi}})^{\text{T}}$, but is itself controlled by the gradients of forces in the expression (3.2) for $\boldsymbol{b}$.

When written out in terms of α and $\boldsymbol{\chi}$, the Riccati relation (2.13) becomes

$$\frac{D\alpha}{Dt} = \chi^2 - \alpha^2 + \alpha_b, \qquad \frac{D\boldsymbol{\chi}}{Dt} = -2\alpha\boldsymbol{\chi} + \boldsymbol{\chi}_b. \tag{4.3}$$

Some years ago, these four equations were first expressed in this form for the incompressible Euler equations without any recourse to quaternions [25]. The quaternionic form first appeared in [8] (see [7]–[9], [28, 29] for a history). Equations (4.3) appear to behave as Lagrangian ODEs driven by $\mathfrak{q}_b = [\alpha_b, \ \boldsymbol{\chi}_b]$. If the latter terms remain roughly constant equations (4.3) can easily be shown to have two fixed points [25]; one has a negative value of α and the other has a positive value. The negative one is associated with an unstable spiral and the positive one with a stable spiral in the phase plane for this simplified ODE system. Equations (4.3) with constant $\mathfrak{q} = [\alpha_b, \ \boldsymbol{\chi}_b]$ have also recently been studied as a remarkably interesting kinematic model for the creation of non-Gaussian statistics in hydrodynamic turbulence [26]. This simple picture would seem not apply if the driving terms $\alpha_b, \ \boldsymbol{\chi}_b$ were to vary on the same timescales as $\alpha, \ \boldsymbol{\chi}$, or faster. This breakdown in applicability of equations (4.3) with constant $\mathfrak{q} = [\alpha_b, \ \boldsymbol{\chi}_b]$ would be indicated if the force gradients in (3.2) were observed to undergo rapid changes.

5. Conclusion

The quaternionic approach to Lagrangian frame dynamics developed here for ICMHD applies generally in fluid dynamics. Because the form of these equations is universal; that is, independent of the specific choice of forces, one may expect them to have many other applications. For example, in MHD one may use these equations to consider the effects on frame dynamics of rotation, or the effects of various kinds of subgrid-scale models, simply by identifying the corresponding expressions for the vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ in equations (2.3) and (2.4). Subgrid-scale models of MHD turbulence may be a particularly fruitful arena for these applications, especially for those models derived from Lagrangian averaging, because Faraday's law for such models is preserved for the averaged field [27]. Depending as it does on Faraday's law, the quaternionic method for MHD is fundamental, but it is also mainly kinematic. Thus its best role may be as a means of developing diagnostics for determining the effects of total force gradients. Therefore, additional applications of the quaternionic approach may also be foreseen, as improved Lagrangian diagnostic methods are developed in the future. For example, future diagnostics may be able to distinguish between effects described by equations (4.3) with fixed values of the quaternion $\mathfrak{q}_b = [\alpha_b, \ \boldsymbol{\chi}_b]$, versus its self-consistent exact dynamics when the vector $\boldsymbol{b}$ is determined from the varying force gradients in equation (3.2).

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