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Automation of The Guiding Center Expansion

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We report on the use of the recently-developed Mathematica package *VEST* (Vector Einstein Summation Tools) to automatically derive the guiding center transformation. Our Mathematica code employs a recursive procedure to derive the transformation order-by-order. This procedure has several novel features. (1) It is designed to allow the user to easily explore the guiding center transformation's numerous non-unique forms or representations. (2) The procedure proceeds entirely in cartesian position and velocity coordinates, thereby producing manifestly gyrogauge invariant results; the commonly-used perpendicular unit vector fields e_1, e_2 are never even introduced. (3) It is easy to apply in the derivation of higher-order contributions to the guiding center transformation without fear of human error. Our code therefore stands as a useful tool for exploring subtle issues related to the physics of toroidal momentum conservation in tokamaks.

I. INTRODUCTION

The guiding center asymptotic expansion is both beautiful and revolting. Its beauty stems from its simple physical underpinning; a strongly magnetized charged particle gyrates around magnetic field lines much more rapidly than it drifts along or across them. This simplicity allows the approximation to be applied in a greater variety of settings than perhaps any other approximation scheme used in magnetized plasma physics. And in spite of the approximation's broad appicability, which might be expected to dilute its power, it affords significant practical benefits. Perhaps most notably, it enables gyrokinetic codes, such as those discussed in Refs. 1 and 2, to work on the drift, rather than gyroperiod, time scale.

The approximation begins to reveal its ugly side, however, when one endeavors to derive successively higher-order contributions to the expansion[3,4]. Aside from the usual proliferation of terms common amongst higher-order perturbation expansions, the obstacles one encounters include vector identities involving spatially varying unit vectors such as $b = \mathbf{B}/|B|$ and subtle issues related to *gyrogauge invariance*[5]. Moreover, attempts to taylor the expansion to respect the Hamiltonian structure of the Lorentz force law encounter the so-called *order-mixing*[4,6] issue, whereby different components of the coordinate transformation one seeks appear at different orders in the transformed Lagrangian, thus complicating the procedure used to find them.

These abhorrent features can be frightening to the uninitiated, meaning only a dedicated minority have ever attempted delving into the calculation beyond the derivation of drifts proportional to first derivatives of the magnetic field. The reluctant majority, up until fairly recently[7], could have justified their stance by proclaiming the higher-order corrections to be practically unimportant, and therefore irrelevant. Recent advances, however, are making it more and more clear that at least corrections proportional to second derivatives of the magnetic field are important for resolving the physics of toroidal momentum conservation in tokamaks[8]. For this reason, certain largely unexplored aspects of these higher-order corrections now appear intriguing to study. In particular, the various *representations* of the guiding center expansion should be explored further.

A representation of the guiding center expansion consists of a prescription for making all of the apparently arbitrary choices one must make in the process of deriving the expansion. Examples of different representations can be found In Ref. 4, where two representations are

presented, or in Littlejohn's work in Refs. 9 and 10. There is nothing unphysical about these different representations - they merely arise from the fact that equations of motion which are independent of gyrophase will remain so upon an arbitrary coordinate transformation that commutes with the gyrosymmetry operation (see appendix B). Nevertheless, different representations lead to guiding center equations of motion with different numbers of terms. Thus, one could imagine optimizing the number of terms in the equations of motion over the space of representations. It is also possible that different representations have different times of validity. After all, Kruskal's method[11], which provides the mathematical basis for the guiding center expansion, can only guarantee equations of motion valid for times of order $1/\epsilon$, where ϵ is the ordering parameter ρ/L[12].

In order to enable the study of these issues, a process which would surely involve deriving the guiding center expansion in many different representations, we have developed, implemented, and verified an algorithm to automate the guiding center calculation using the newly-developed Mathematica package *VEST* (Vector Einstein Summation Tools)[13]. In particular, we have slashed the time required to derive the expansion, and all but eliminated the possible taint of human-made algebra errors in the derivation of higher-order contributions to the guiding center expansion.

While other authors have presented algorithmic procedures for deriving the guiding center expansion in the past[4,14,15], the algorithm we present here is novel due to the combination of the following.

1) The algorithm *has actually been implemented on a computer* and used to derive the guiding center expansion in two different representations.

2) Complicated, multi-term, vector identities are accounted for using the clever simplification capabilities of *VEST*.

3) Issues related to gyrogauge invariance are completely avoided by working in cartesian position and velocity coordinates. In particular, the only unit vector that plays a role is the physical $b = \mathbf{B}/|B|$.

4) Gyroaverages and Fourier expansions in gyrophase are implemented in these coordinates using a coordinate-independent formulation of these operations.

5) The approach manages to be manifestly Hamiltonian while addressing the order-mixing issue in a computationally attractive manner; for each $m > n$, the n'th-order contribution to the perturbative coordinate transformation is determined without knowledge of any of

the details of the m'th order contribution.
6) The manner in which we address the order-mixing issue obviates the high degree of freedom in the form of the transformed Lagrangian.

In what follows, we will describe our algorithm and report on the equations of motion generated in the two representations just alluded to. We will begin with four sections describing what our algorithm is meant to do as well as our motivation for selecting an algorithm with the novel features just described. In section II, we give a schematic overview of Hamiltonian Lie transform-based perturbation theory in order to remind the reader of the goal of the guiding center expansion. We then describe the motivation for selecting our algorithm via a description of three difficulties we faced while developing it, and how we overcame them. In particular, sections III, IV, and V are devoted to discussing the difficulties presented by the order-mixing issue; the desire for manifestly gyrogauge invariant results; and the task of computing gyroaverages and gyroharmonics, respectively. With all of the motivations in place, we present our algorithm in section VI. Finally, in section VII, we present the results of automatically performing the guiding center expansion with our algorithm in two previously unstudied representations.

II. A SCHEMATIC FOR HAMILTONIAN LIE TRANSFORM PERTURBATION THEORY

In this section, we will review the general structure and purpose of the guiding center expansion, and thereby indicate precisely what our algorithm is meant to do. We then discuss three key difficulties we faced while trying to develop the algorithm before actually presenting presenting it. The purpose of these four sections is to provide a narrative explaining why the algorithm looks the way it does. Readers only interested in the algorithm itself can skip straight to section VI, but it may still be useful to skim these early sections in order to become familiar with our notation.

We begin by recalling the coordinate-independent formulation of Hamiltonian dynamical systems[16]. This formulation makes use of Cartan's exterior calculus of differential forms; a very brief overview of the latter is provided in Appendix A. The phase space M is assumed to be an even dimensional smooth manifold[17] equipped with a symplectic two-form ω. The dynamical equations are then specified by a function $H : M \to \mathbb{R}$ known as the Hamiltonian

function via Hamilton's equations

$$\mathrm{i}_{X_H}\omega = \mathbf{d}H, \tag{1}$$

where X_H is the vector field that specifies the time derivative of any particle's phase space location $c(t) \in M$, i.e. $c'(t) = X_H(c(t))$. In any local coordinate system (z^i) on M, Hamilton's equations become

$$\dot{z}^i \omega_{ij} = \frac{\partial H}{\partial z^j}, \tag{2}$$

where $\dot{z}^i$ are the components of the vector field $X_H = \dot{z}^i \frac{\partial}{\partial z^i}$ and $\omega_{ij} = \omega(\frac{\partial}{\partial z^i}, \frac{\partial}{\partial z^j})$.

In the guiding center problem, the phase space is the six-dimensional position-velocity space, $M = \mathbb{R}^3 \times \mathbb{R}^3$, equipped with the symplectic form $\omega_\epsilon = -\mathbf{d}\vartheta_\epsilon$, where the one-form ϑ_ϵ is given in terms of the the magnetic vector potential $\mathbf{A}$ and the guiding center ordering parameter ϵ by

$$\vartheta_\epsilon = \mathbf{A} \cdot dx + \epsilon v \cdot dx. \tag{3}$$

The equations of motion are then specified by the Hamiltonian function $H = \frac{1}{2}\epsilon^2 v \cdot v$. As can be readily verified, the vector field $X_H(\epsilon)$ in the natural cartesian coordinates on M is given by

$$\begin{aligned} \dot{v}(x,v) &= v \times \mathbf{B}(x) \\ \dot{x}(x,v) &= \epsilon v. \end{aligned} \tag{4}$$

Strictly speaking, the placement of the ordering parameter $\epsilon = \rho/L$ in ϑ_ϵ, and therefore its placement in the equations of motion, is only justified in appropriate dimensionless variables, as discussed in Ref. 3. However, we can regard Eq. (4) as a dimensional equation if we think of ϵ as a formal ordering parameter and if we normalize $\mathbf{A}$ by a particle's charge-to-mass ratio so that $\mathbf{B}$ has the dimension of frequency.

When $\epsilon = 0$, which corresponds to the asymptotic limit where a particle undergoes gyromotion with zero gyroradius and vanishingly slow drift, the equations of motion given in Eq. (4) are gyrosymmetric[18,19] (see section IV for the precise definition of gyrosymmetric tensors). Because the particle trajectories are periodic in this limit, Kruskal's general theory[11] tells us that we can asymptotically deform, or rearrange, the phase space M using a non-unique ϵ-dependent near-identity transformation $T_\epsilon : M \to M$ such that the transformed $X_H(\epsilon)$, $X_H(\epsilon') \equiv T_{\epsilon *} X_H(\epsilon)$, is gyrosymmetric to *all orders in* ϵ.

The goal of the guiding center theory, and therefore the algorithm we will present later, is to find such a T_ϵ. Because performing this task requires a degree of ingenuity, a number of useful methods have been developed. Of particular relevance to the present work are those methods that employ Lie transforms. In these cases, one posits that the desired transformation from the old phase space to the new, deformed phase space can be expressed in the form[20]

$$T_\epsilon = ... \circ \exp(-G_n(\epsilon)) \circ ... \circ \exp(-G_1(\epsilon)), \tag{5}$$

where, for each n, $G_n(\epsilon) : M \to TM$ is a vector field that tends to zero as $\epsilon \to 0$, and does so more rapidly than does $G_m(\epsilon)$ with $m < n$. The requirement that the transformed equations of motion be gyrosymmetric then reduces to a sequence of requirements on the $G_n(\epsilon)$. Thus, the Lie transform approach to finding T_ϵ reduces to finding a sequence of $G_n(\epsilon)$ that satisfy the latter requirements.

One can derive these requirements in one of two ways. The direct method, which recently made an appearance in Ref. 21 (also see Ref. 22), consists of formally computing the transformed $X_H(\epsilon)$, $X'_H(\epsilon) = T_{\epsilon *} X_H(\epsilon)$, using Eq. (5) and then demanding that the result be gyrosymmetric to all orders. The Hamiltonian method, due to Littlejohn[23], consists of calculating the transformed $\mathbf{d}\vartheta_\epsilon$ and H, $T_{\epsilon *}\mathbf{d}\vartheta_\epsilon$ and $T_{\epsilon *}H$, and then demanding that each of be gyrosymmetric to all orders. These two methods are related by the general fact that if the ω and H appearing in Hamilton's equations (1) admit a symmetry, then so does X_H. Each method also involves making a number of arbitrary decisions to completely determine the $G_n(\epsilon)$; different choices lead to different representations.

In principle, either approach can be automated on a computer. Indeed, historically this has been one of the advertised "features" of the Lie transform approach to perturbation problems in general. However, the Hamiltonian approach has the advantage of automatically providing the Hamiltonian structure of the equations of motion in the new arrangement of phase space. It is for this reason that we pursue the Hamiltonian approach in the present work.

III. DIFFICULTY 1: ORDER-MIXING

While developing the algorithm for automating the Hamiltonian Lie transform approach to finding T_ϵ, we encountered three key difficulties. In this section and the two that follow

we will describe each in turn, as well as the manner in which we overcame each difficulty.

The first issue is rooted in the special form of ϑ_ϵ given above. If one specifies the ϵ-dependence of the $G_n(\epsilon)$ according to $G_n(\epsilon) = \epsilon^n g_n$, then the one-form ϑ_ϵ on the deformed phase space is given by

$$\vartheta'_\epsilon = \mathbf{A} \cdot dx + \epsilon v \cdot dx + \epsilon L_{g_1}(\mathbf{A} \cdot dx) + O(\epsilon^2), \tag{6}$$

where L_{g_1} denotes the Lie derivative with respect to the vector field g_1 (see appendix A). In order to find one of the transformations guaranteed by Kruskal's theory, the combination $v \cdot dx + L_{g_1}(\mathbf{A} \cdot dx)$ must be gyrosymmetric, modulo closed one-forms[24]. If we write $g_1 = g_1^x \cdot \frac{\partial}{\partial x} + g_1^v \cdot \frac{\partial}{\partial v}$, this condition can be satisfied by choosing $g_1^x = \frac{1}{|B|} v \times b$, $g_1^v =$ anything. However, as would become clear upon analyzing higher-order contributions to the transformed one-form, there are in fact constraints on g_1^v that destroy the apparent complete freedom in its specificaiton. This is a special case of the more general order-mixing issue; the various components of any given vector field g_n appear at different orders in ϑ'_ϵ.

From a computational point of view, order-mixing is bothersome. It obfuscates the extent to which the choices one needs to make to find the various g_n are coupled across n-values. If the coupling were severe enough, then any algorithm one might construct to automate these choices could be very complicated.

In order to overcome this difficulty, we designed our algorithm to satisfy

Resolution of Difficulty 1: The rule for determining $G_n(\epsilon)$ does not rely on any specific knowledge of any component of $G_m(\epsilon)$ whenever $m > n$.

In section VI, the precise manner in which the algorithm accomplishes this will become clear.

IV. DIFFICULTY 2: MANIFEST GYROGAUGE INVARIANCE

In order to understand the second difficulty we faced in developing a good algorithm for automating the guiding center calculation, one needs to understand the usual definition of a gyrosymmetric tensor. This definition refers to a special type of coordinate system on M, any instance of which we will call a *fibered coordinate system*. A fibered coordinate system

on M consists of an open subset $U \subset M$, 5 smooth functions $\xi^i : U \to \mathbb{R}$, $i = 1, ..., 5$, and one additional function $\theta : U \to \mathbb{R} \bmod 2\pi$ satisfying:

F1[25]: The six functions ξ_i, $i = 1, ..., 5$, and θ define a valid coordinate system on U

F2: Holding the ξ_i fixed, θ parameterizes, in a left-handed sense relative to b, the zero'th order ($\epsilon = 0$) solutions to Eq. (4), which are called *loops* by Kruskal.

The standard example of a family of fibered coordinate systems used in guiding center theory is constructed as follows. First find a smooth unit vector field e_1 perpendicular to the magnetic field, $e_1 \cdot b = 0$. $e_1(x)$ and $e_2(x) = (b \times e_1)(x)$ span the plane perpendicular to $b(x)$ for each x in the domain of definition, $D \subset \mathbb{R}^3$, of e_1, as depicted in Figure 1. As shown in Ref. 18, D cannot always be taken to be the entire 3-dimensional domain particles move through. A fibered coordinate system can then be defined on the open subset of phase space $U \equiv \{(x, v) \in M | x \in D \text{ and } b(x) \times v \neq 0\}$. Labeling the ξ_i according to $(\xi_1, \xi_2, \xi_3) = x$, $\xi_4 = v_\perp$, $\xi_5 = v_\parallel$, these functions are defined by the relation

$$\begin{aligned} x =& x(x, v) \\ v =& v_\parallel(x, v) b(x) \\ &+ v_\perp(x, v) \left(\cos(\theta(x, v)) e_1(x) - \sin(\theta(x, v)) e_2(x)\right). \end{aligned} \tag{7}$$

A gyrosymmetric tensor can then be defined in terms of fibered coordinate systems as follows. A tensor is gyrosymmetric if its components in an arbitrary fibered coordinate system do not depend on θ. Note that one doesn't have to look at a tensor in every fibered coordinate system to check this property; it is enough to check in a collection of fibered coordinate systems that cover M.

This standard definition of gyrosymmetric tensors motivates the standard approach to deriving the constraints on the $G_n(\epsilon)$. One first writes out the components of the transformed $\mathbf{d}\vartheta_\epsilon$ and H in a family of fibered coordinate systems on M that cover M. Then one chooses the local representatives of $G_n(\epsilon)$ to eliminate the θ-dependence in these components in each coordinate system in the covering. For consistency, one also must demand that the local definitions of $G_n(\epsilon)$ agree when changing from one fibered coordinate system in the covering

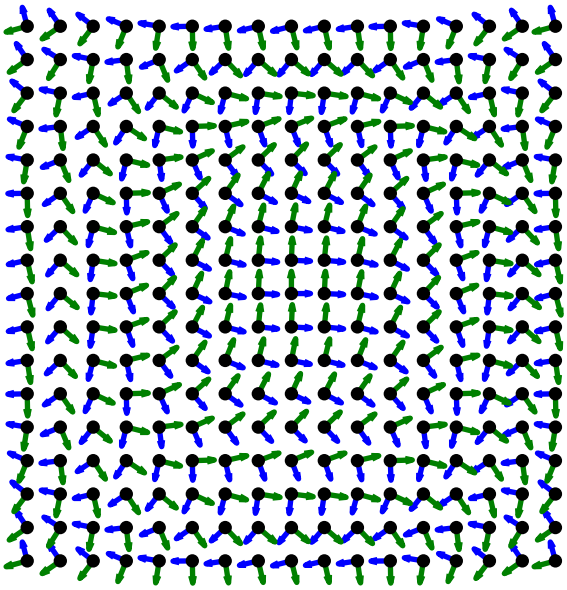

FIG. 1. A typical arrangement of the perpendicular unit vectors e_1, e_2 for a uniform magnetic field that points out of the page. The two sets of arrows represent e_1 and e_2. While in this case, e_1 and e_2 are not *required* to vary in space, for a more general sort of magnetic field, they would be.

to another. The latter is one statement of the principle of gyrogauge invariance.

There is nothing conceptually wrong with this approach to finding the $G_n(\epsilon)$, and it can be made to work. However, there is a very practical problem with proceeding in precisely this manner on a computer. In order to verify that a given expression for $G_n(\epsilon)$ in a fibered coordinate system constructed using some perpendicular unit vector e_1 satisfies the principle of gyrogauge invariance, it is often necessary to account for non-trivial vector identities involving the perpendicular unit vectors e_1 and b. Presently, there is no general method that would allow one to do this on a computer in all cases one might encounter. Thus, one cannot guarantee that the $G_n(\epsilon)$ produced by a computer following the above procedure will *manifestly* exhibit gyrogauge invariance, i.e. it will not be obvious that $G_n(\epsilon)$ is gyrogauge invariant, even if it actually is.

In order to avoid this issue, we have chosen to avoid using fibered coordinate systems altogether.

Resolution of Difficulty 2: All tensors are expressed and manipulated in cartesian posi-

tion and velocity coordinates.

By proceeding in this manner, the results generated by our algorithm ($G_n(\epsilon)$, for example) will be expressed entirely in terms of v, $|B|$, b, and derivatives thereof, thereby making our algorithm manifestly gyrogauge invariant; perpendicular unit vectors e_1, e_2 and the gyrophase coordinate θ are never even introduced.

V. DIFFICULTY 3: COORDINATE-INDEPENDENT FOURIER ANALYSIS

The third issue we wish to discuss arises as a result of our resolution of the difficulty discussed in the previous section. If we demand that all tensors be expressed and manipulated in cartesian coordinates, then how can we check if a given tensor is gyrosymmetric? Moreover, how can we compute the gyroaverage and gyroharmonics of a tensor in these coordinates?

A conceptually appealing way to answer these questions is to first derive some coordinate-independent properties of the gyrosymmetry that would allow one to answer these questions in an arbitrary coordinate system, and then specialize to cartesian coordinates. To our knowledge, this interesting mathematical exercise has not been discussed elsewhere in the literature, and so we will provide the details in the remainder of this section.

First notice that in a fibered coordinate system (ξ_i, θ) (this is shorthand for the sextuplet $(\xi_1, ..., \xi_5, \theta)$), a function $f : U \to \mathbb{R}$ is gyrosymmetric if and only if

$$f(\xi_i, \theta + \psi) = f(\xi_i, \theta) \tag{8}$$

for all constants ψ. If, for each $\psi \in \mathbb{R} \bmod 2\pi$, we define the mapping $\Phi_\psi : U \to U$ using the formula

$$\Phi_\psi(\xi_i, \theta) = (\xi_i, \theta + \psi), \tag{9}$$

then the condition given in Eq. (8) can be re-expressed as

$$\Phi_\psi^* f = f \tag{10}$$

for each $\psi \in \mathbb{R} \bmod 2\pi$. Here Φ_ψ^* denotes the pullback operator on functions, $\Phi_\psi^* f = f \circ \Phi_\psi$.

While the formula (8) only makes literal sense in a fibered coordinate system, the family of mappings Φ_ψ can actually be given a coordinate independent definition. Indeed, in cartesian position and velocity coordinates we have[26]

$$\begin{aligned}&\Phi_\psi(x,v) = \\ &(x, v\cdot b(x)b(x) + \cos(\psi)b(x)\times(v\times b(x)) + \sin(\psi)v\times b(x)).\end{aligned} \tag{11}$$

Thus, gyrosymmetric functions $f : M \to \mathbb{R}$ can be alternately characterized as those functions that satisfy the analogue of Eq. (10), $\Phi_\psi^* f = f$ for each $\psi \in \mathbb{R} \bmod 2\pi$.

What about more general tensor fields? Because the pullback operator of a mapping $M \to M$ is well defined on the entire tensor algebra, it is tempting to postulate that a tensor field τ is gyrosymmetric if and only if $\Phi_\psi^*\tau = \tau$ for all $\psi \in \mathbb{R} \bmod 2\pi$. This is indeed correct; it is a straightforward exercise to verify that this characterization is equivalent to the usual one stated in the previous section.

What is going on here? If we fix a $\psi \in \mathbb{R} \bmod 2\pi$, then the mapping $\Phi_\psi : M \to M$ can be regarded as a global rearrangement, or relabeling, of points in M. If we regard Φ_ψ as pointing from the "new arrangement" to the "old arrangement", then $\Phi_\psi^*\tau$ is nothing more than τ, regarded as a tensor in the old arrangement of M, expressed in the new arrangment. Thus, from this point of view, we see that gyrosymmetric tensors are precisely those tensors whose form is invariant under any of the rearrangments in the family Φ_ψ.

With this coordinate independent characterization of gyrosymmetric tensors in hand, we now seek a corresponding coordinate-independent version of Fourier analysis in the gyrophase θ. The catch is that we do not desire to work with the gyrophase coordinate θ directly as the latter is only defined in fibered coordinate systems. Instead we will use the parameter ψ in the family of maps Φ_ψ as a surrogate of sorts.

Given an arbitrary tensor τ, set $\tau_\psi = \Phi_\psi^*\tau$. τ_ψ can be regarded as a periodic tensor field-valued function of the single variable ψ with period 2π. Therefore it admits a Fourier expansion

$$\tau_\psi = \langle\tau\rangle + \sum_{k=1}^{\infty}(\Pi_k\tau)\cos(\psi) + (\bar{\Pi}_k\tau)\sin(\psi), \tag{12}$$

where the tensor fields $\langle\tau\rangle$, $\Pi_k\tau$, and $\bar{\Pi}_k f$ are given by

$$\begin{aligned}\langle\tau\rangle &= \frac{1}{2\pi}\int_0^{2\pi}(\Phi_\psi^*\tau)d\psi \\ \Pi_k\tau &= \frac{1}{\pi}\int_0^{2\pi}(\Phi_\psi^*\tau)\cos(k\psi)d\psi \\ \bar{\Pi}_k\tau &= \frac{1}{\pi}\int_0^{2\pi}(\Phi_\psi^*\tau)\sin(k\psi)d\psi.\end{aligned} \tag{13}$$

Note that $\Pi_k\tau$ and $\bar{\Pi}_k\tau$ are not gyrosymmetric tensors. Instead they satisfy the identities

$$\begin{aligned}\Phi_\psi^*(\Pi_k\tau) &= \cos(k\psi)(\Pi_k\tau) + \sin(k\psi)(\bar{\Pi}_k\tau) \\ \Phi_\psi^*(\bar{\Pi}_k\tau) &= -\sin(k\psi)(\Pi_k\tau) + \cos(k\psi)(\bar{\Pi}_k\tau).\end{aligned} \tag{14}$$

However, as the notation suggests, $\langle\tau\rangle$ is indeed gyrosymmetric.

The Fourier inversion formula, Eq. (13), together with the invariance properties given in Eq. (14), is sufficient to solve all of the linear partial differential equations that one encounters while deriving expressions for the $G_n(\epsilon)$ in any coordinate system. Thus, we have effectively solved the problem of performing Fourier analysis in θ in cartesian position and velocity coordinates without ever referring to fibered coordinate systems. We have incorporated this solution into our algorithm as

Resolution of Difficulty 3: Gyroaverages and gyroharmonics are calculated in cartesian position and velocity coordinates using Eqs. (13) and (14).

VI. THE ALGORITHM

As discussed in section II, the goal of the algorithm is to find a transformation T_ϵ in the form given in Eq. 5 such that $T_{\epsilon*}\mathbf{d}\vartheta_\epsilon$ and $T_{\epsilon*}H$ are each gyrosymmetric to all orders in ϵ (section IV gives the general definition of a gyrosymmetric tensor). This T_ϵ consists of a concatenated sequence of transformations of the form $\exp(Y)$. Thus, we are free to think of T_ϵ as the result of many intermediate transformations, each closer to the identity transformation than the last. Our algorithm proceeds by finding expressions for these intermediate transformations (which amounts to specifying a $G_n(\epsilon)$), one at a time, according to the following recursive procedure.

Suppose that some finite number of intermediate transformations have been performed. Let Θ_ϵ and $\mathcal{H}_\epsilon$ denote the resulting one-form and Hamiltonian following this partial rearrangement of M, and assume they have the form:

$$\begin{aligned}\Theta_\epsilon =&\vartheta_0 + \epsilon\vartheta_1 + ... + \epsilon^N\vartheta_N + \sum_{k=1}^{\infty}\epsilon^{N+k}\alpha_k \\ \mathcal{H}_\epsilon =&H_0 + ... + \epsilon^{N-2}H_{N-2} + \sum_{k=1}^{\infty}\epsilon^{N-2+k}h_k,\end{aligned} \tag{15}$$

where $N > 1$, the ϑ_j and H_j are all gyrosymmetric, and the α_j and h_j are not necessarily so. Suppose further that $\Xi_\epsilon = \vartheta_0 + ... + \epsilon^N\vartheta_N$ satisfies the three properties

ND1[27]: $\mathbf{d}\Xi_\epsilon$ is a non-degenerate two-form.

ND2: If β is an ϵ-independent one-form, then the vector field $Y(\epsilon)$ defined by $\mathrm{i}_{Y(\epsilon)}\mathbf{d}\Xi_\epsilon = \beta$ (i.e. Y is the application of the Poisson tensor defined by Ξ_ϵ to β) is $O(\epsilon^{-2})$.

ND3: When $\beta = -\mathbf{d}H_0$, the leading order behavior of $Y(\epsilon)$ is given by $\frac{|B|}{\epsilon^2}\xi \equiv \frac{|B|}{\epsilon^2}v \times b \cdot \frac{\partial}{\partial v}$.

In this setting, which will serve as our inductive assumption, it is possible to find a transformation $\exp(-G(\epsilon))$, for some small vector field $G(\epsilon)$, such that after this transformation, the one-form and the Hamiltonian have the same form as in Eq. (15), but with N replaced with $N+1$, i.e. the one-form and Hamiltonian are each gyrosymmetric to one higher order than previously. This also means that the transformed Ξ_ϵ will automatically continue to satisfy properties ND1-3. We will call a $G(\epsilon)$ that produces a transformation $\exp(G(\epsilon))$ with the latter two properties a *recursive* vector field.

To see that one can in fact find *many* recursive vector fields under the inductive assumption, let $G(\epsilon)$ be a vector field that solves the algebraic equation (see appendix C for a solution method)

$$\mathrm{i}_{G(\epsilon)}\mathbf{d}\Xi_\epsilon + \epsilon^{N+1}\alpha_1 + \epsilon^{N+1}\mathbf{d}S = \mathrm{i}_{\langle G(\epsilon)\rangle}\mathbf{d}\Xi_\epsilon + \epsilon^{N+1}\langle\alpha_1\rangle, \tag{16}$$

where S is the unique function with $\langle S\rangle = 0$ (see section V for the definition of the general tensor gyroaverage operator $\langle\rangle$) that solves the partial differential equation (see appendix D

for a solution method)

$$h_1 - |B|\mathrm{i}_\xi \alpha_1 - |B|\mathrm{i}_\xi \mathbf{d}S = \langle h_1 \rangle - |B|\mathrm{i}_\xi \langle \alpha_1 \rangle . \tag{17}$$

Note that the oscillatory part of $G(\epsilon)$, $\tilde{G}(\epsilon) = G(\epsilon) - \langle G(\epsilon) \rangle$, is then uniquely determined, but the gyroaverage $\langle G(\epsilon) \rangle$ is left completely free. Constrain the latter so that it satisfies

$$\mathrm{i}_{\langle G(\epsilon) \rangle} \mathbf{d}\Xi_\epsilon = \epsilon^{N+1} \gamma, \tag{18}$$

where γ is any ϵ-independent gyrosymmetric one-form.

As is readily verified, such a $G(\epsilon)$ satisfies the following important properties.

P1: $G(\epsilon) = O(\epsilon^{N-1})$, but will be a rational function of ϵ.

P2: Upon applying the transformation $\exp(-G(\epsilon))$, the transformed one-form (modulo closed one-forms) and Hamiltonian, Θ'_ϵ and $\mathcal{H}'_\epsilon$, become

$$\begin{aligned} \Theta'_\epsilon =& \vartheta_0 + ... + \epsilon^N \vartheta_N \\ &+ \epsilon^{N+1} \left(\langle \alpha_1 \rangle + \gamma \right) + O(\epsilon^{N+2}), \end{aligned} \tag{19}$$

and

$$\begin{aligned} \mathcal{H}'_\epsilon =& H_0 + ... + \epsilon^{N-2} H_{N-2} \\ &+ \epsilon^{N-1} \left(\langle h_1 \rangle + |B|\mathrm{i}_\xi \gamma \right) + O(\epsilon^N). \end{aligned} \tag{20}$$

Thus, the entire family of $G(\epsilon)$ just defined, a family which may be regarded as being parameterized by the arbitrary gyrosymmetric one-form γ, consists of recursive vector fields.

With these recursive vector fields in hand, all that we must now show is that there is some base case, consisting of a one-form and Hamiltonian in the form specified by Eq. (15), from which our recursive algorithm can start. Unfortunately this base case clearly cannot be the natural choice, $\Theta_\epsilon = \mathbf{A} \cdot dx + \epsilon v \cdot dx$ and $\mathcal{H}_\epsilon = \frac{1}{2}\epsilon^2 v \cdot v$, as this pair is not in the form specified by Eq. (15). However, this issue is easy to resolve. First, notice that if the transformed $\frac{1}{\epsilon^2} H$ is gyrosymmetric, then H will be too. Therefore, remove the ϵ^2 from the Hamiltonian. Second, recognize that we are free to perform a preparatory transformation before finding the $G_n(\epsilon)$. In particular, we can apply a preparatory near-identity transformation of the

form $\exp(-\epsilon G_0)$ that transforms $\mathcal{H}_\epsilon = \frac{1}{2} v \cdot v$ and $\Theta_\epsilon = \mathbf{A} \cdot dx + \epsilon v \cdot dx$ into the form specified by Eq. (15) with $N = 2$. For instance, with

$$\begin{aligned} G_0 = & -\frac{v \times b}{|B|} \cdot \frac{\partial}{\partial x} \\ & + \left(\frac{(v \cdot b) \nabla b \cdot (b \times v)}{|B|} + \frac{(v \times b) \cdot \nabla b \cdot v b}{2|B|} \right. \\ & \left. + \frac{(v \cdot b)(b \cdot \nabla \times b) b \times (v \times b)}{|B|} \right) \cdot \frac{\partial}{\partial v} \end{aligned} \tag{21}$$

then we arrive at the satisfactory starting point

$$\begin{aligned} \Theta_\epsilon &= \mathbf{A} \cdot dx + \epsilon (v \cdot b) b \cdot dx \\ &+ \frac{1}{2|B|} \epsilon^2 \left(v \times b \cdot dv - (v \cdot b)[\nabla b \cdot (v \times b)] \cdot dx \right) + O(\epsilon^3) \\ \mathcal{H}_\epsilon &= \frac{1}{2} v \cdot v + O(\epsilon). \end{aligned} \tag{22}$$

To summarize, our algorithm for finding the $G_n(\epsilon)$ that generate T_ϵ proceeds as follows.

1: Because any real calculation can only calculate a finite number of the $G_n(\epsilon)$, when one stops calculating additional $G_n(\epsilon)$, the one-form and Hamiltonian will be of the form specified in Eq. (15) with $N = N_{\max}$. Therefore, specify the desired $N_{\max}$.

2: Define three integers N, M, and l with initializations $N = 2$, $M = N_{\max} - 2$, and $l = 1$.

3: Apply a preparatory transformation, such as that given in Eq. (21), so that the one-form and Hamiltonian have the form specified in Eq. (15). Only the first M non-gyrosymmetric terms must be calculated in each case.

4: Find a recursive vector field $G_l(\epsilon)$. Use Eq. (16) to find the unique oscillatory part $\tilde{G}_l(\epsilon)$, and specify the gyroaveraged part $\langle G_l(\epsilon) \rangle$ using an arbitrary gyrosymmetric one-form γ_l according to Eq. (18).

5: Store $G_l(\epsilon)$. Set $l = l + 1$, $N = N + 1$, and $M = M - 1$.

6: Using the recursive vector field just derived to specify the transformation, express the new one-form and Hamiltonian in the form specified in Eq. (15). Only the first M non-gyrosymmetric terms must be calculated in each case.

7: If $N = N_{\max}$, stop. Else, return to step *4*.

Note that different representations of the guiding center expansion will be generated for each choice of the sequence of gyrosymmetric one-forms γ_l. In particular, if one does not attempt to constrain the form of the transformed Hamiltonian, the $O(\epsilon^3)$ contribution to the transformed one-form can be any gyrosymmetric one-form whatsoever, including 0. Likewise, if one does not attempt to constrain the form of the transformed one-form, then the $O(\epsilon)$ contribution to the transformed Hamiltonian can be specified arbitrarily (at least away from those points in phase space where $v \times b = 0$).

Finally, note that the presence of a preparatory transformation implies that the complete transformation from the old phase space to the new, deformed phase space is given by $T_\epsilon \circ \exp(-\epsilon G_0)$, with $T_\epsilon = ... \circ \exp(-G_2(\epsilon)) \circ \exp(-G_1(\epsilon))$.

VII. TWO NEW REPRESENTATIONS

To illustrate the use of our algorithm, we now turn to presenting the results of using it to derive two previously unexplored representations of the guiding center expansion. Each representation we present here will choose $\gamma_l + \langle \alpha_1 \rangle = 0$ in step *4*, meaning each representation is closely related to the so-called Hamiltonian representation discussed in Ref. 4. The two representations will differ in which preparatory transformation is used in step *3*.

In each case, we will provide explicit expressions for the transformed one-form accurate to all orders in ϵ. For the transformed Hamiltonians, we will provide H_0, H_1, and H_2. This information is enough to accurately express the transformed equations of motion up to and including terms of order ϵ^2. For the sake of brevity, we will not specify the $G_n(\epsilon)$. However, we stress that, when equipped with a copy of our code, finding these vector fields that specify the transformation would be a simple task for any interested reader. In fact, each of the results below takes about fifteen minutes to derive on a laptop computer. We would also like to stress that all of the following results have been checked directly by calculating how the

one-form and Hamiltonian transform according to the $G_n(\epsilon)$ we derived and indirectly by verifying that we reproduce the well-known first-order correction to the magnetic moment adiabatic invariant, μ_1 (see Ref. 28, for example):

$$\begin{aligned}\mu_1 = \frac{1}{|B|^2}\Bigg(&\frac{1}{4}v\cdot\nabla b\cdot(v\times b)(v\cdot b) \\ &-\frac{3}{4}(v\times b)\cdot\nabla b\cdot v(v\cdot b)-\frac{5}{4}b\times\kappa\cdot v(v\cdot b)^2 \\ &+\frac{1}{2|B|}(v\times b)\cdot(v\times b)\nabla|B|\times b\cdot v\Bigg).\end{aligned} \tag{23}$$

Moreover, while we have not performed a direct comparison of our μ_2 to existing expressions, we have verified that the μ_2 predicted by the $G_n(\epsilon)$ in each representation agree with one another.

Example 1:

This representation will be defined by the use of the preparatory transformation already given in Eq. (21) and by always choosing $\gamma_l + \langle\alpha_1\rangle = 0$. The consequences of these choices come in the form of a transformed one-form equal to that given in Eq. (22), thus simplifying the form of the transformed Poisson bracket. In fact, by expressing Eq. (22) in the usual sort of fibered coordinate system, we see

$$\Theta_\epsilon = \mathbf{A}\cdot dx + \epsilon v_\parallel b\cdot dx + \epsilon^2\mu[d\theta - \mathbf{R}\cdot dx], \tag{24}$$

where $\mu = \frac{v_\perp^2}{2|B|}$ and $\mathbf{R} = (\nabla e_1)\cdot e_2$, meaning the transformed Poisson bracket is exactly the

same as that given in Ref. 5. Meanwhile the transformed Hamiltonian is given by

$$
\begin{aligned}
H_0 =& \frac{1}{2} v \cdot v \\
H_1 =& \frac{1}{2} (v \cdot b) \mu \tau \\
H_2 =& \mu^2 \Bigg(\frac{15}{16} (\nabla \cdot b)^2 + \frac{1}{16} \kappa \cdot \kappa + \frac{1}{4} b \cdot \nabla (\nabla \cdot b) \\
& - \frac{1}{16} \mathrm{tr}[\nabla b \cdot \nabla b + \nabla b \cdot (\nabla b)^T] \\
& - \frac{3}{4} \nabla \ln |B| \cdot \nabla \ln |B| + \frac{1}{4} \kappa \cdot \nabla \ln |B| + \frac{1}{4|B|} \nabla^2 |B| \Bigg) \\
& + \mu \frac{(v \cdot b)^2}{|B|} \Bigg(\frac{1}{8} \mathrm{tr}[3 \nabla b \cdot \nabla b - \nabla b \cdot (\nabla b)^T] + \frac{1}{8} (\nabla \cdot b)^2 \\
& \qquad + \frac{1}{2} b \cdot \nabla (\nabla \cdot b) + \frac{13}{8} \kappa \cdot \kappa - \frac{3}{2} \kappa \cdot \nabla \ln |B| \Bigg) \\
& - \frac{(v \cdot b)^4}{|B|^2} \Bigg(\frac{1}{2} \kappa \cdot \kappa \Bigg)
\end{aligned}
\tag{25}
$$

where $\mu = \frac{(v \times b) \cdot (v \times b)}{2|B|}$, $\tau = b \cdot \nabla \times b$, and $\kappa = b \cdot \nabla b$. Note that the H_2 in this representation differs from the H_2 in Brizard and Tronko's Hamiltonian representation[4] (also see Ref. 6), although it is similarly complicated. In order to recover the latter representation, it would be necessary to choose $\langle \alpha_1 \rangle + \gamma_l = \mathbf{d} f_l$ with appropriately chosen f_l.

Example 2:

The second representation will also make the choice $\gamma_l + \langle \alpha_1 \rangle = 0$, but the preparatory transformation $\exp(-\epsilon G_0)$ will be specified by

$$
\begin{aligned}
G_0 = & -\frac{v \times b}{|B|} \cdot \frac{\partial}{\partial x} + \frac{1}{|B|} \Bigg((v \cdot b)(v \times b) \cdot \nabla b \\
& - 2 (v \cdot b) \nabla b \cdot (v \times b) + \frac{1}{4} v \cdot [\nabla b + \nabla b^T] \cdot (v \times b) b \\
& \qquad + \frac{3}{4} b \cdot \kappa \times v (v \cdot b) b \Bigg) \cdot \frac{\partial}{\partial v}
\end{aligned}
\tag{26}
$$

This implies that the transformed one-form is given by

$$
\begin{aligned}
\Theta_\epsilon &= \mathbf{A} \cdot dx + \epsilon (v \cdot b) b \cdot dx \\
&+ \frac{1}{2|B|} \epsilon^2 \Bigg(v \times b \cdot dv - (v \cdot b) [\nabla b \cdot (v \times b)] \cdot dx - \mu |B| \tau b \cdot dx \Bigg) \\
&= \mathbf{A} \cdot dx + \epsilon v_\parallel b \cdot dx + \epsilon^2 \mu [d\theta - (\mathbf{R} + \frac{1}{2} \tau b) \cdot dx].
\end{aligned}
\tag{27}
$$

Thus, the transformed Poisson bracket is the same as that given in Ref. 6. The transformed Hamiltonian is given by

$$H_0 = \frac{1}{2} v \cdot v \tag{28}$$

$$H_1 = 0 \tag{29}$$

$$\begin{aligned} H_2 = \mu^2 \Bigg(& \frac{15}{16}(\nabla \cdot b)^2 + \frac{3}{16}\kappa \cdot \kappa + \frac{1}{4} b \cdot \nabla(\nabla \cdot b) \\ & + \frac{1}{16}\mathrm{tr}[\nabla b \cdot \nabla b - 3\nabla b \cdot (\nabla b)^T] \\ & - \frac{3}{4}\nabla \ln |B| \cdot \nabla \ln |B| + \frac{1}{4}\kappa \cdot \nabla \ln |B| + \frac{1}{4|B|}\nabla^2 |B| \Bigg) \\ + \mu \frac{(v \cdot b)^2}{|B|} \Bigg(& \frac{1}{8}\mathrm{tr}[3\nabla b \cdot \nabla b - \nabla b \cdot (\nabla b)^T] + \frac{1}{8}(\nabla \cdot b)^2 \\ & + \frac{1}{2} b \cdot \nabla(\nabla \cdot b) + \frac{13}{8}\kappa \cdot \kappa - \frac{3}{2}\kappa \cdot \nabla \ln |B| \Bigg) \\ - \frac{(v \cdot b)^4}{|B|^2} & \left(\frac{1}{2}\kappa \cdot \kappa \right). \end{aligned}$$

VIII. DISCUSSION

We have reported, for the first time, on the automatic calculation of the guiding center expansion using a computer. In particular, we have implemented a novel Lie transform-based algorithm using the newly-developed Mathematica package *VEST*[13] and used it to derive two new representations of the guiding center equations of motion to the order relevant for studying issues related to the physics of toroidal momentum conservation in tokamaks. By proceeding in this manner, we have avoided the pitfalls associated with hand-made algebra errors and slashed the time required to perform the calculations from weeks to minutes. Readers interested in obtaining the Mathematica notebook week used to carry out our calculation can contact J. Squire via email at jsquire@princeton.edu.

There are a number of opportunities for extending this work. Because our algorithm provides the necessary tools to explore many representations of the guiding center expansion, it may be interesting to begin searching through different representations to find those with desirable properties such as simple transformed equations of motion. Likewise, it may be interesting to examine the time-validity of the transformed equations of motion in these different representations to see if some are worse than others. Kruskal's theory[11] guarantees $1/\epsilon$ time-validity in all representations, but there may be representations that can do better.

Yet another suitable application of our code would be pushing the calculation to higher order than previously calculated. For instance, it would be interesting to find μ_3 and H_3. Finally, there should be no great difficulty in extending both our algorithm and our implementation in Mathematica using *VEST* to treat the gyrocenter transformation theory that forms the backbone of modern gyrokinetic theory.

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Appendix A: Elements of Exterior Calculus

In this appendix we will first list the basic identities commonly used when performing calculations with the exterior calculus. Then we will give the component-form of the basic operators $\mathbf{d}$, L_Y, i_Y in the velocity phase space. For a much more thorough treatment of this topic, refer to Ref. 16.

Let α_k and β_l be k- and l-forms on the manifold M, respectively. Let Y and Z be vector fields on M. Then the following identities hold

$$\alpha_k \wedge \beta_l = (-1)^{kl} \beta_l \wedge \alpha_k \tag{A1}$$

$$\mathrm{i}_Y(\alpha_k \wedge \beta_l) = (\mathrm{i}_Y \alpha_k) \wedge \beta_l + (-1)^k \alpha_k \wedge (\mathrm{i}_Y \beta_l) \tag{A2}$$

$$\mathbf{d}(\alpha_k \wedge \beta_l) = (\mathbf{d}\alpha_k) \wedge \beta_l + (-1)^k \alpha_k \wedge (\mathbf{d}\beta_l) \tag{A3}$$

$$L_Y(\alpha_k \wedge \beta_l) = (L_Y \alpha_k) \wedge \beta_l + \alpha_k \wedge (L_Y \beta_l) \tag{A4}$$

$$\mathrm{i}_Y \mathrm{i}_Z = -\mathrm{i}_Z \mathrm{i}_Y \tag{A5}$$

$$L_Y = \mathbf{d}\mathrm{i}_Y + \mathrm{i}_Y \mathbf{d} \tag{A6}$$

$$\mathbf{d} L_Y = L_Y \mathbf{d} \tag{A7}$$

$$\mathbf{d}\mathbf{d} = 0. \tag{A8}$$

Let $F : M \to M$ and $\Phi : M \to M$ be smooth mappings with a smooth inverses F^{-1} and Φ^{-1}. One example of this sort of mapping from the main text is Φ_ψ, for fixed ψ, whose

inverse is $\Phi_{-\psi}$. The exterior calculus operations behave very well with respect to mappings. We will summarize this fact with a second list of identities.

$$F^*\Phi^* = (\Phi \circ F)^* \tag{A9}$$

$$F^*(\alpha_k \wedge \beta_l) = (F^*\alpha_k) \wedge (F^*\beta_l) \tag{A10}$$

$$F^*(\mathrm{i}_Y \alpha_k) = \mathrm{i}_{F^*Y}(F^*\alpha_k) \tag{A11}$$

$$F^*(L_Y \alpha_k) = L_{F^*Y}(F^*\alpha_k) \tag{A12}$$

$$F^*(\mathbf{d}\alpha_k) = \mathbf{d}(F^*\alpha_k). \tag{A13}$$

When $F = \exp(Y(\epsilon))$, with $Y(\epsilon)$ a vector field that tends to zero as $\epsilon \to 0$, we also have the asymptotic identities

$$\exp(-Y(\epsilon))_*\tau = \exp(Y(\epsilon))^*\tau \tag{A14}$$

$$\exp(Y(\epsilon))^*\tau = \tau + L_{Y(\epsilon)}\tau + \frac{1}{2}L^2_{Y(\epsilon)}T + ..., \tag{A15}$$

where τ is an arbitrary tensor.

The identities provided thus far, together with the fact that the wedge product is associative, are sufficient to verify all of the coordinate-independent manipulations of differential forms in the main text. In order to perform exterior calculus using *VEST* it is also useful to have component-based expressions for the operators $\mathbf{d}$, i_Y, and L_Y. Actually, the relevant operators for the sake of performing the guiding center calculation are $\mathbf{d}$ on functions, i_Y on one-forms, and $\mathrm{i}_Y\mathbf{d}$ on both functions and one-forms.

Let $Y = Y^{xi}\frac{\partial}{\partial x^i} + Y^{vi}\frac{\partial}{\partial v^i}$, where the indices are summed from $i = 1$ to $i = 3$ (although we do so by habit, there is really no need to distinguish between covariant and contravariant indices in cartesian coordinates). Similarly, let $\alpha = \alpha_{xi}dx^i + \alpha_{vi}dv^i$. Denote derivatives of a scalar f with respect to the i'th spatial argument and the i'th velocity argument with $f_{,i}$

and $f_{;j}$, respectively (note that ; does *not* denote a covariant derivative). Then we have

$$\mathbf{d}f = f_{,i}dx^i + f_{;i}dv^i \tag{A16}$$

$$\mathrm{i}_Y\alpha = \alpha_{xi}Y^{xi} + \alpha_{vi}Y^{vi} \tag{A17}$$

$$\mathrm{i}_Y\mathbf{d}f = f_{,i}Y^{xi} + f_{;i}Y^{vi} \tag{A18}$$

$$\begin{aligned}\mathrm{i}_Y\mathbf{d}\alpha = {} & (\alpha_{xi,j} - \alpha_{xj,i})Y^{xj}dx^i \\ & + (\alpha_{xi;j}Y^{vj} - \alpha_{vj,i}Y^{xj})dx^i \\ & + (\alpha_{vi,j}Y^{xj} - \alpha_{xj;i}Y^{xj})dv^i \\ & + (\alpha_{vi;j} - \alpha_{vj;i})Y^{vj}dv^i.\end{aligned} \tag{A19}$$

Note that, by the identity given in Eq. (A6), the Lie derivative of a one-form, $L_Y\alpha = \mathbf{d}\mathrm{i}_Y\alpha + \mathrm{i}_Y\mathbf{d}\alpha$, can also be calculated using these component expressions.

Appendix B: The Origin of Many Representations of The Guiding Center Expansion

Suppose that a near-identity rearrangement of the phase space $T_\epsilon : M \to M$ is found that renders the transformed Lorentz vector field $X'_H = T_{\epsilon *}X_H$ gyrosymmetric. As explained by Kruskal[11], at least one such transformation can be found using perturbation theory. In fact, as soon as one transformation in found, many more can be generated easily. This implies that there is much freedom in choosing T_ϵ; each choice leads to a different representation of the guiding center equations of motion in the sense that X'_H will be different in each case. In this appendix we will explain the origin of this freedom by completely characterizing it.

First note that if $F : M \to M$ is a rearrangement of phase space (not necessarily near-identity) that commutes with the family of rearrangements Φ_ψ that define the gyrosymmetry (see section V), i.e. $F \circ \Phi_\psi = \Phi_\psi \circ F$ for each $\psi \in \mathbb{R} \bmod 2\pi$, then $X''_H \equiv F_*X'_H$ is also gyrosymmetric. Indeed,

$$\begin{aligned}\Phi^*_\psi X''_H &= \Phi_{-\psi *}F_*X'_H \\ &= (\Phi_{-\psi} \circ F)_*X'_H \\ &= (F \circ \Phi_{-\psi})_*X'_H \\ &= F_*\Phi^*_\psi X'_H = X''_H,\end{aligned} \tag{B1}$$

where we have used the fact that X'_H is gyrosymmetric and $F \circ \Phi_\psi = \Phi_\psi \circ F$. This tells us that, given one of the near-identity rearrangements of phase space guaranteed by Kruskal, we can find many more by following the latter with any near-identity rearrangement of phase space that commutes with Φ_θ.

In fact *all* of the rearrangements that fit into Kruskal's theory can be found in this manner. To be precise, suppose that $R_\epsilon : M \to M$ and $Q_\epsilon : M \to M$ are two near identity rearrangements that render X_H gyrosymmetric, so that they fit into Kruskal's theory. Then, by definition, $\Phi^*_\psi(R_{\epsilon *} X_H) = R_{\epsilon *} X_H$ and $\Phi^*_\psi(Q_{\epsilon *} X_H) = Q_{\epsilon *} X_H$. Thus, both Q_ϵ and R_ϵ define symmetry transformations on the original arrangement of phase space, $\bar{\Phi}^Q_\psi = Q^{-1}_\epsilon \circ \Phi_\psi \circ Q_\epsilon$ and $\bar{\Phi}^R_\psi = R^{-1}_\epsilon \circ \Phi_\psi \circ R_\epsilon$ that leave X_H invariant. Kruskal has proven in Ref. 11 that these two symmetry transformations are in fact identical to all orders in ϵ; $\bar{\Phi}_\psi \equiv \bar{\Phi}^Q_\psi = \bar{\Phi}^R_\psi$. It follows then that the rearrangement $F = Q_\epsilon \circ R^{-1}_\epsilon$ commutes with Φ_ψ. But this is precisely the rearrangement that sends $R_{\epsilon *} X_H$ into $Q_{\epsilon *}$, which tells us that each representation of the guiding center equations of motion can be reached from a given one by applying a near-identity transformation that commutes with Φ_θ.

Note that if a rearrangement of the form $\exp(Y)$, for some vector field Y, commutes with Φ_θ, then it must be true that $Y = \langle Y \rangle$. This is why one should expect complete freedom to choose the $\langle G_n(\epsilon) \rangle$ for each $G_n(\epsilon)$ appearing in the Lie transform ansatz given in Eq. (5).

Appendix C: A General Formula For Inverting Exact Lagrange Tensors Defined On The Velocity Phase Space

Step *4* in our algorithm involves solving an algebraic equation of the form $\mathrm{i}_X \mathbf{d}\Xi = -\beta$ for the vector field X given a non-degenerate two-form $\mathbf{d}\Xi$ and an arbitrary one-form β. In this appendix we will present explicit expressions for the components of $X = X^{xi}\frac{\partial}{\partial x^i} + X^{vi}\frac{\partial}{\partial v^i}$ in terms of the components of $\Xi = A_i dx^i + B_i dv^i$ and $\beta = \beta_{xi} dx^i + \beta_{vi} dv^i$.

We proceed by making use of the linear isomorphism between the space of vector fields and the space of five-forms induced by the Liouville volume form

$$\Omega = \frac{1}{6} \mathbf{d}\Xi \wedge \mathbf{d}\Xi \wedge \mathbf{d}\Xi. \tag{C1}$$

This isomorphism is given by $X \mapsto \mathrm{i}_X \Omega$. One can easily prove that this is an isomorphism using the fact that the non-degeneracy of $\mathbf{d}\Xi$ implies that Ω is nowhere vanishing. The

reason this isomorphism is useful is that it is easier to find $\mathcal{X} \equiv \mathrm{i}_X\Omega$ than X. Indeed, upon wedge multiplying $\mathbf{d}\Xi \wedge \mathbf{d}\Xi$ into both sides of the equation $\mathrm{i}_X\mathbf{d}\Xi = -\beta$, we obtain

$$\mathcal{X} = -\frac{1}{2}\mathbf{d}\Xi \wedge \mathbf{d}\Xi \wedge \beta. \tag{C2}$$

By explicitly calculating the right hand side of the last expression in components, and then inverting the isomorphism $X \mapsto \mathrm{i}_X\Omega$, we obtain

$$\begin{aligned} X^{xn} =& -\frac{1}{\mathcal{D}}\Bigg(\epsilon^{ilk}\epsilon^{mjn}\beta_{xm}B_{k;l}(B_{i,j} - A_{j;i}) \\ &+ \epsilon^{lkm}\epsilon^{jin}\beta_{vm}A_{i,j}B_{k;l} \\ &+ \frac{1}{2}\epsilon^{kim}\epsilon^{jln}\beta_{vm}(B_{i,j} - A_{j;i})(B_{k,l} - A_{l;k})\Bigg) \end{aligned} \tag{C3}$$

$$\begin{aligned} X^{vn} =& \frac{1}{\mathcal{D}}\Bigg(\epsilon^{jil}\epsilon^{kmn}\beta_{vm}A_{i;j}(B_{k,l} - A_{l;k}) \\ &+ \epsilon^{mji}\epsilon^{lkn}\beta_{xm}A_{i,j}B_{k;l} \\ &+ \frac{1}{2}\epsilon^{mjl}\epsilon^{kin}\beta_{xm}(B_{i,j} - A_{j;i})(B_{k,l} - A_{l;k})\Bigg), \end{aligned} \tag{C4}$$

where the function $\mathcal{D}$ is defined by the relation $\Omega = \mathcal{D}dx^1 \wedge dx^2 \wedge dx^3 \wedge dv^1 \wedge dv^2 \wedge dv^3$.

Appendix D: Solving The Equation for S

In order to complete step *4* in our algorithm, the partial differential equation

$$h_1 - |B|\mathrm{i}_\xi\alpha_1 - |B|\mathrm{i}_\xi\mathbf{d}S = \langle h_1\rangle - |B|\mathrm{i}_\xi\langle\alpha_1\rangle \tag{D1}$$

must be solved for S given $|B|$, α_1, h_1, and the constraint $\langle S\rangle = 0$. As is readily verified by gyroaveraging the equation, an equivalent condition on S is that it be chosen to eliminate the non-zero gyroharmonics of the quantity $h_1 - |B|\mathrm{i}_\xi\alpha_1 - |B|\mathrm{i}_\xi\mathbf{d}S$.

Let $\nu = h_1 - |B|\mathrm{i}_\xi\alpha_1$. Using Eq. (13), we see that the Fourier expansion of $\nu_\psi = \Phi_\psi^*\nu$ is given by

$$\nu_\psi = \langle\nu\rangle + \sum_{k=1}^{\infty}\Pi_k\nu\cos(k\psi) + \bar{\Pi}_k\nu\sin(k\psi). \tag{D2}$$

Using the identities $L_\xi\Pi_k S = k\bar{\Pi}_k S$ and $L_\xi\bar{\Pi}_k S = -k\Pi_k S$, we also see that the Fourier expansion of $\Phi_\psi^*|B|\mathrm{i}_\xi\mathbf{d}S = |B|L_\xi S_\psi$ is given by

$$|B|L_\xi S_\psi = \sum_{k=1}^{\infty}|B|k\bar{\Pi}_k S\cos(k\psi) - |B|k\Pi_k S\sin(k\psi). \tag{D3}$$

Therefore, S must be given by

$$S = \sum_{k=1}^{\infty} \Pi_k S \tag{D4}$$
$$= \sum_{k=1}^{\infty} -\frac{\bar{\Pi}_k \nu}{|B|k}.$$

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[20]For some quick intuition regarding this ansatz, recall that the time-advance map associated to an arbitrary vector field $Y : M \to TM$ is given by $\exp(tY)$. Thus, given $x \in M$, $T_\epsilon(x)$ is found by sequentially flowing along the vector fields $G_n(\epsilon)$ for -1 unit of time each, starting from x.

[21]V. M. L. De Guillebon, (2013), arXiv:1211.5792.

[22]N. Bogoliubov, *Asymptotic Methods in the Theory of Non-Linear Oscillations*, International monographs on advanced mathematics and physics (Hindustan, 1961).

[23]R. G. Littlejohn, J. Math. Phys. **23**, 742 (1982).

[24]Demanding the transformed $\mathbf{d}\vartheta_\epsilon$ to be gyrosymmetric is equivalent to demanding that the transformed ϑ_ϵ be equal to the sum of a gyrosymmetric one-form and an arbitrary closed one-form. This follows from the fact that $\mathbf{d}\vartheta'_\epsilon$ is left unchanged upon replacing ϑ'_ϵ with $\vartheta'_\epsilon + \alpha$ for an arbitrary closed one-form α, i.e. $\mathbf{d}\alpha = 0$.

[25]F stands for "fibered".

[26]In spite of its simplicity and utility, this formula only seems to have been noticed recently. It can be found in the literature in Ref. 18. It was also independently discovered by Zhi Yu[29], but never published.

[27]ND stands for "non-degenerate".

[28]B. Weyssow and R. Balescu, J. Plasma Phys. **35**, 449 (1986).

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