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Gyrosymmetry: global considerations

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In the guiding center theory, smooth unit vectors perpendicular to the magnetic field are required to define the gyrophase. The question of global existence of these vectors is addressed using a general result from the theory of principal circle bundles. It is found that there is, in certain cases, an obstruction to global existence. In these cases, the gyrophase cannot be defined globally. The implications of this fact on the basic structure of the guiding center theory are discussed. In particular it is demonstrated that the guiding center asymptotic expansion of the equations of motion can still be performed in a globally consistent manner when a single global convention for measuring gyrophase is unavailable. The key to this demonstration is thinking of the asymptotic expansion as leveraging the globally defined zero'th order symmetry associated to the magnetic moment.

I. INTRODUCTION

There is no doubt that the Hamiltonian formulation of guiding center theory is a foundational aspect of modern gyrokinetic theories. Simply put, it provides a means for deforming the single-particle phase space so as to illuminate the approximate symmetry associated to the magnetic moment, the gyrosymmetry, while keeping the Hamiltonian structure of the particle dynamics in focus. However, in spite of its importance and the number of years it has been studied¹⁻¹², there are still poorly understood subtleties in the theory.

In this paper, we study the subtleties associated with the so-called “perpendicular unit vectors” that make an appearance in virtually every version of the theory^{1-11,13}. These quantities, hereafter referred to as e_1 and e_2 , are *smooth* unit vector fields everywhere perpendicular to the magnetic field and to one another, meaning they form an orthonormal triad together with $b = B/||B||$ in the velocity space. From one point of view, they appear in the formalism for the sake of identifying an angular variable θ , the gyrophase, that evolves on a fast timescale with respect to the evolution timescale of the remaining dynamical variables, thereby putting the guiding center problem in the setting of the generalized method of averaging described in Ref. 13. In particular, when the equations of motion for a strongly magnetized charged particle are expressed using a cylindrical parameterization of velocity space such that the cylindrical axis points along the magnetic field, then it can be shown that the polar angle associated to this cylindrical coordinate system furnishes such a fast angle. This angle is measured with respect to a pair of mutually orthogonal normalized vectors e_1, e_2 lying in the plane perpendicular to B . Because the magnetic field varies spatially, e_1, e_2 must also vary in space so as to accommodate the constraint $e_1 \cdot B = 0$. Therefore these e_1, e_2 furnish an example of perpendicular unit vectors (see Fig. 1). From another, more geometric point of view, the perpendicular unit vectors usher themselves into the formalism so as to facilitate parameterizing the zero’th-order symmetry loops, or Kruskal Rings¹⁴⁻¹⁶ associated with the gyrosymmetry; one of the vectors, say e_1 , distinguishes a point on each Kruskal Ring which then serves as a reference or zero angle. Interestingly, nobody’s version of the theory ever provides a general, constructive definition of these e_1, e_2 in terms of known quantities. This is the first hint that there is more to these vector fields than meets the eye.

Perhaps the reason nobody provides such a definition is that, in the most general setting where the guiding center expansion applies, e_1, e_2 simply cannot be defined globally, that is,

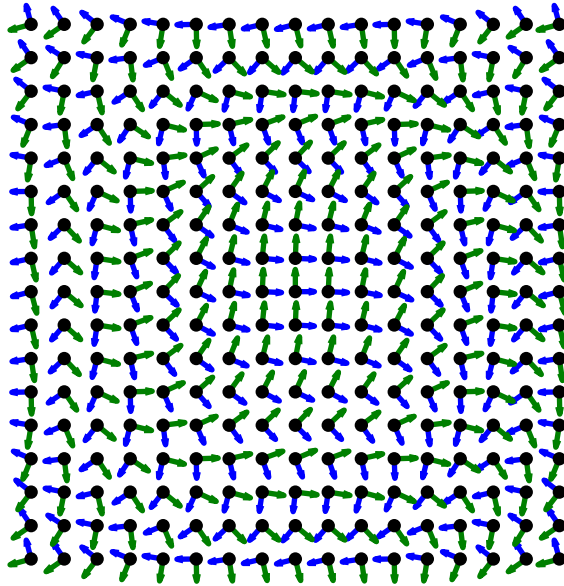


FIG. 1. A typical arrangement of the perpendicular unit vectors e_1, e_2 for a uniform magnetic field that points out of the page. The two sets of arrows represent e_1 and e_2 . While in this case, e_1 and e_2 are not *required* to vary in space, for a more general sort of magnetic field, they would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

there might not even be one vector field defined over the *entire* configuration space that is at once perpendicular to B and of unit length. While it is easy to see that smooth e_1, e_2 can always be defined *locally* in some, generally tiny, open neighborhood of any point p in the configuration space¹⁷, this in no way implies that these locally defined perpendicular unit vectors extend to well-defined global quantities^{18–20}. So could there be an obstruction the global existence of smooth e_1, e_2 in some cases?

If we take this question seriously, a more important one arises immediately. Is the guiding center theory still valid without global perpendicular unit vectors? As the theory is carried out to higher order, expressions involving the perpendicular unit vectors and their derivatives appear in the equations of motion; see Ref. 3 for instance. So it might seem plausible that the existence of global equations of motion is tied to the global properties of e_1, e_2 .

Here we will put both of these questions to rest. We will provide a complete mathematical description of the obstruction to global perpendicular unit vectors and show that this obstruction does not always vanish. However, we demonstrate that the obstruction does indeed vanish if the physical domain is an open solid torus. Then we will show that the

guiding center theory *does* provide consistent global equations of motion in the absence of global e_1, e_2 owing to the fact that the symmetry associated with the magnetic moment is always globally defined. To illustrate this second point, we provide an expression for the guiding center Poincaré-Cartan one-form in terms of globally defined physical quantities like B ; neither the perpendicular unit vectors nor the gyrophase appear in the expression.

The paper is structured as follows. In II we provide a simple example of a magnetic field that does not admit global e_1, e_2 . Then in III, we provide a complete mathematical description of the obstruction to global perpendicular unit vectors in the most general case. As an example illustrating the theory, we prove in IV that if the physical domain²¹, D , particles are tracked through is an open, solid torus, then it is always possible to find global e_1, e_2 . This is even true when the magnetic field lines are chaotic! Then we give a non-trivial example of a magnetic field that does not admit global e_1, e_2 . Finally in V, we show that the guiding center theory *does* provide consistent global equations of motion in the absence of global e_1, e_2 .

II. A MOTIVATING EXAMPLE: THE FIELD DUE TO A MAGNETIC MONOPOLE

The field due to a magnetic monopole provides probably the simplest illustration of the obstruction to the existence of global e_1, e_2 . Perhaps the simplicity comes at the cost of physical relevance, but the latter will be reclaimed later after developing some machinery. Amusingly, the possibility that this example *is* physically relevant has never been ruled out. See Ref. 22 for an interesting discussion of the current status of magnetic monopoles in theoretical physics.

The monopole field is given by

$$B(x) = \frac{1}{||x||^2} e_r(x), \quad (1)$$

where e_r is the radial unit vector from a spherical coordinate system about the origin. It is depicted in Fig. 2. Sufficiently far from the singularity at the origin, we could in principle develop the guiding center approximation. So let the physical domain D where particles would move consist of the open region exterior to some sphere of radius r_o centered on the origin. Now let's see if there is a perpendicular unit vector defined on all of D .

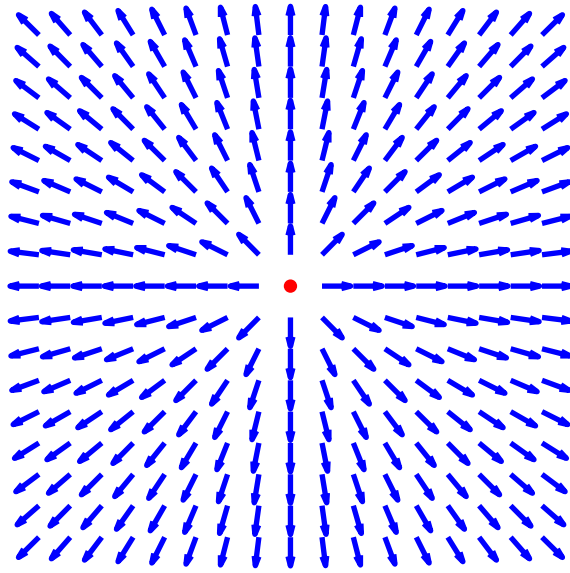


FIG. 2. The magnetic field due to a magnetic monopole. Note that $\nabla \cdot B = 0$ except at the origin, which is depicted as a large central dot.

If there were such a vector field, e_1 , then it could be restricted to a sphere centered on the origin with radius $r_a > r_o$, S_{r_a} . Because $B|_{S_{r_a}}$ is parallel to the vector normal to S_{r_a} , $e_1|_{S_{r_a}}$ would have to be everywhere tangent to S_{r_a} . Thus,

$$e_1|_{S_{r_a}} : S_{r_a} \rightarrow TS_{r_a},$$

where TS_{r_a} denotes the tangent bundle²³ of S_{r_a} , would furnish an example of a smooth non-vanishing tangent vector field on the sphere. But this situation is impossible by the famous “hairy ball theorem”. It follows that no such e_1 exists.

There are two essential features of this example. First of all, notice that D has a “hole” due to excluding the region with $r < r_o$. If instead D were chosen to be some solid spherical region separated from the singularity at the origin, then it *would* be possible to find an e_1 (we won’t prove this now). But then D would be hole free. So we see that the obstruction to the existence of e_1 is related to the topology of D . Second, consider the structure of the “hairy ball” argument. Define the magnetic circle bundle, SD , to be the collection of circles $SD_x \subseteq T_x D$, where for each $x \in D$, SD_x consists of all those vectors emanating from x that are perpendicular to $B(x)$ and unit length. The argument really worked because of the way SD is arranged. In particular, note that even if D had holes, if SD arose from a uniform

magnetic field, then there would certainly exist globally defined perpendicular unit vectors. So the global “twisting” of the perpendicular planes is a relevant aspect to the obstruction to global e_1, e_2 .

III. THE GENERAL OBSTRUCTION TO GLOBAL PERPENDICULAR UNIT VECTORS

Now we will generalize the important aspects of the previous example to completely determine the conditions for the existence of global e_1, e_2 in the most general setting. Namely, we want to determine when a nowhere vanishing magnetic field defined on some three dimensional open set $D \subseteq \mathbb{R}^3$, admits a globally smoothly defined perpendicular unit vector e_1 .

The appropriate way to tackle this problem is to recognize that SD is actually a principal circle bundle and that the existence of a globally defined perpendicular unit vector is equivalent to the existence of a global section of SD (see appendix A for the necessary background on principal circle bundles). Because a principal circle bundle admits a global section if and only if it is a trivial bundle, the existence problem can be solved by appealing to the well-established topological classification of principal circle bundles²⁴. This classification theorem tells us that if we can find any so-called principal connection on SD (see appendix B for the necessary background on principal connections), which is a special sort of one-form over SD , then the curvature of this connection, a closed two-form over D induced by the principal connection, will be exact if and only if SD is a trivial bundle. Thus, given the curvature form, existence of global perpendicular unit vectors can be tested by integrating the curvature form over a collection of cycles that generate D 's second homology group $H_2(D, \mathbb{Z})$ ²⁵. If all of these integrals vanish, then the curvature form must be exact and a global section of SD must exist.

So in order to furnish a solution to the existence problem, all that we must still do is 1) prove that SD is a principal circle bundle whose global sections, if they exist, coincide with global perpendicular unit vectors and 2) derive an expression for the curvature form associated to some principal connection on SD . Then existence can be determined in any particular case after finding the “holes” in D .

First notice that SD is indeed a manifold. Actually it is a submanifold of $TD = D \times \mathbb{R}^3$

defined by the algebraic equations

$$\begin{aligned} v \cdot v &= 1 \\ v \cdot b(x) &= 0, \end{aligned} \tag{2}$$

where $(x, v) \in TD$. Next, consider the following circle action on SD :

$$\Phi_\theta(x, v) = (x, \exp(\theta \hat{b}(x)) v), \tag{3}$$

where $\hat{b}(x)$ is the 3×3 antisymmetric matrix defined by $\hat{b}(x)w = b(x) \times w$, and \exp denotes the matrix exponential. Hence this circle action simply rotates all of the circles that comprise SD by θ radians. Furthermore, the action is free. Therefore (SD, Φ) forms a principal circle bundle.

To see that the sections of this circle bundle are equivalent to the perpendicular unit vectors, we first show that the base space of the bundle can be identified with D . Define the map $\pi : SD \rightarrow D$ by

$$\pi(x, v) = x. \tag{4}$$

π is a surjective submersion and $\pi^{-1}(x)$ is equal to the circle in SD over x , which is an entire orbit of the action Φ . It follows that $SD/S^1 = D$ with π serving as the bundle projection map. Thus a global section of SD would consist of a smooth map of the form $s : D \rightarrow SD$ with the property $\pi(s(x)) = x$, that is, $s(x)$ must lie in the circle over x . Because all of the points on the circle over x are by definition perpendicular to $b(x)$ and of unit length, s would be a global perpendicular unit vector. Conversely, any global perpendicular unit vector would define such an s .

Now we move on to define a principal connection on SD . Because it will be necessary to work with the space $TSD \subseteq TTD$, we make the following identification:

$$TTD = T(D \times \mathbb{R}^3) = TD \times T\mathbb{R}^3 = (D \times \mathbb{R}^3) \times (\mathbb{R}^3 \times \mathbb{R}^3).$$

Accordingly, a typical element of the 12 dimensional space TTD will be denoted (x, u, v, a) , where (u, a) forms the tangent vector over the point $(x, v) \in TD$. Clearly, each element of TSD can also be written in this way (of course u and a will be constrained in this case). It will also be helpful to define a metric on TD . Recall that such a metric on TD defines an

inner product on each of the tangent spaces in TTD . The useful metric in this case assigns an inner product to each $(x, v) \in TD$ given by

$$\left\langle (x, u, v, a), (x, u', v, a') \right\rangle = u \cdot u' + a \cdot a'. \quad (5)$$

Note the distinction between this inner product denoted by square brackets and the usual dot product between vectors in \mathbb{R}^3 . Finally, a principal connection $\mathcal{A} : TSD \rightarrow \mathbb{R}$ can be defined by

$$\mathcal{A}(x, u, v, a) = \left\langle (x, u, v, a), (x, 0, v, b(x) \times v) \right\rangle = a \cdot b(x) \times v. \quad (6)$$

The two defining properties of a principal connection (appendix B) are straightforward to check.

Next we derive an expression for the curvature form associated to \mathcal{A} . Because a local section $s_\alpha : U_\alpha \subseteq D \rightarrow \pi^{-1}(U_\alpha)$ must be of the form

$$s_\alpha(x) = (x, e_1(x)), \quad (7)$$

where e_1 is a locally defined perpendicular unit vector, the gauge fields must be of the form

$$\begin{aligned} A_\alpha(x, w) &= s_\alpha^* \mathcal{A}(x, w) = \left(w \cdot \nabla e_1(x) \right) \cdot b(x) \times e_1(x) \\ &\equiv w \cdot R(x). \end{aligned} \quad (8)$$

As the notation suggests, $R = (\nabla e_1) \cdot b \times e_1 = (\nabla e_1) \cdot e_2$ is the well-known quantity that appears elsewhere in the guiding center formalism. Therefore, the curvature form $F = dA_\alpha$ is given by the equation

$$*F = N \cdot dx, \quad (9)$$

where $*$ is the hodge star and $N = \nabla \times R$. By the transformation law for curvature forms given in appendix B, N must be a globally defined quantity even when e_1 , and therefore R , is not. In fact, there is an expression giving N in terms of b ^{3,4}:

$$\begin{aligned} N &= \frac{1}{2} b \left(\text{Tr}(\nabla b \cdot \nabla b) - (\nabla \cdot b)^2 \right) \\ &\quad + (\nabla \cdot b) b \cdot \nabla b - b \cdot \nabla b \cdot \nabla b. \end{aligned} \quad (10)$$

With (10) in hand, all of the tools required to determine the existence of global perpendicular unit vectors have been assembled. To reiterate, to test for existence, the curvature

form F should be integrated over a collection of cycles that generate D 's second homology group $H_2(D, \mathbb{Z})$. Intuitively, this amounts to calculating the flux of N through a collection of closed, bounded, boundary-less surfaces that encapsulate the “holes” in D . If all of these integrals vanish, then there will be global perpendicular unit vectors. Otherwise, owing to the ensuing non-trivial topology of SD , global perpendicular unit cannot be defined, even in principle. Notice that this question of the existence of perpendicular unit vectors is quite similar to the question of the existence of a globally defined vector potential outside of a magnetic monopole. The topological properties of principal bundles play a fundamental role in each case.

IV. SOME EXAMPLE ASSESSMENTS OF THE EXISTENCE OF GLOBAL PERPENDICULAR UNIT VECTORS

Now we will apply the machinery developed in the previous section to assess the existence of global perpendicular unit vectors for a few example choices of D and B . Because of their relevance to magnetic confinement, we will first treat the broad class of examples where D is an open solid torus and B is only constrained to be non-vanishing on D . We will show that, in these examples, global perpendicular unit vectors can always be found. Then we will consider a more exotic example where B is linear and vanishes at a single point and D is taken to be the region surrounding the field null. In this case global perpendicular unit vectors do *not* exist.

When D is an open solid torus, for instance the region contained within the vacuum vessel of a tokamak device, then its second homology group $H_2(D, \mathbb{Z})$ vanishes. This is because D is homotopic to the circle, the homology groups are homotopy invariants, and the circle has a vanishing second homology group. Putting this fact intuitively, there are no boundary-less 2-dimensional surfaces contained in D that enclose a hole. It follows then that every boundary-less 2-dimensional surface contained in D arises as the boundary of some 3-dimensional region. Stoke's theorem then implies that, because $\nabla \cdot N = 0$, the flux of N through any such surface must vanish. Therefore we arrive at the following conclusion: when D is an open solid torus, global perpendicular unit vectors always exist.

It is worth mentioning that this conclusion holds even when there are chaotic magnetic field lines. To see that this is reasonable, consider a typical tokamak field that has been

subjected to a resonant magnetic perturbation. Often, for instance in Ref. 26, these perturbations are not large enough to completely kill the toroidal component of the magnetic field at any point within the last closed flux surface (assume this region is D). However, it is well known that they may nonetheless create regions of chaotic field lines. Therefore, in spite of the presence of chaotic field lines, the vector

$$E_1 = e_R \times B = B_\phi e_z - B_z e_\phi, \quad (11)$$

where e_R, e_ϕ are the cylindrical radial and azimuthal unit vectors, vanishes nowhere in D and so defines a global perpendicular unit vector $e_1 = E_1/||E_1||$. Similarly “X-points” and “O-points” lead to no obstruction to a global e_1, e_2 .

Now consider the magnetic field given by

$$B(x, y, z) = ye_x + ze_y + xe_z. \quad (12)$$

Let $D = \mathbb{R}^3 \setminus \{0\}$. Thus we only exclude from D the one point where B vanishes. Note that there is nothing singular about B at 0 even though b is. Also note that the current density $\nabla \times B$ is uniform. It is straightforward to compute the flux of N through a sphere of any radius centered on the origin, which turns out to be -4π . This implies immediately that there cannot exist global perpendicular unit vectors on D .

Interestingly, a corollary to this last result is that D cannot be foliated into toroidal magnetic flux surfaces, else a global e_1 could be defined as the surface normal to the flux surfaces. In fact this will be true any time global perpendicular unit vectors fail to exist. However, as the first example showed, the implication does *not* go the other way; the lack of flux surfaces does not necessarily imply an obstruction to the existence of global e_1, e_2 .

V. HOW THE GUIDING CENTER THEORY WORKS WITHOUT GLOBAL PERPENDICULAR UNIT VECTORS

When a perpendicular unit vector cannot be defined globally, the usual notion of gyrophase loses its global meaning as well. So what happens to the guiding center perturbation expansion? Because D can always be covered by (perhaps tiny) open regions U_α in which *local* e_1, e_2 are defined, the perturbation procedure can certainly be carried out in each of these patches. The result of each of these local calculations would then consist of

formal phase space coordinate changes given as formal one-to-one maps $\phi_\alpha : U_\alpha \times \mathbb{R}^3 \rightarrow \mathbb{R}^6$ that lead to simpler equations of motion in the new coordinates. However, these coordinate changes will not necessarily fit together to define a global coordinate change, i.e. an invertible mapping of the entire phase space into itself. Therefore, when calculating the motion of a particle as it moves from one U_α to the next, it becomes necessary to occasionally pass the mechanical state from one ϕ_α to another in order to continue using the simplified equations of motion provided by the perturbation theory. While this can be done formally by developing expressions for $\phi_\alpha \circ \phi_\beta^{-1}$, practically it would involve truncating asymptotic series each time the particle crossed from one U_α to the next. This could lead to coherently accumulating error in a simulation, and, in general, would destroy the Hamiltonian properties of the simplified equations of motion.

A far better approach is to look for a global change of coordinates to accomplish the perturbation theory *from the outset*. This way the mess associated with truncating the expansions of the $\phi_\alpha \circ \phi_\beta^{-1}$ could be avoided altogether. We will show that such a global coordinate change can be found for the guiding center problem owing to the fact that the zero'th order symmetry is globally defined. We will do this by applying a version of Lie perturbation theory to the guiding center problem that synthesizes Littlejohn's Poincaré-Cartan one-form approach developed in Ref. 27 (also see Ref. 28) with the group-theoretic structure provided by a zero'th order symmetry. Littlejohn's formalism provides a means for performing the perturbation expansion in each of the regions of phase space where the perpendicular unit vectors can be defined, while the globally defined symmetry serves as the needle that sews these local calculations into a global result.

For simplicity we will only consider the time-independent case. To begin, the guiding center phase space is $P = D \times \mathbb{R}^3 \times \mathbb{R}$. The first factor corresponds to the physical domain particles move through, the second is the velocity space, and the third is the time axis. Denote a typical element of this phase space by (x, v, t) and a typical element of $TP = TD \times T\mathbb{R}^3 \times T\mathbb{R}$ by (u_x, a_v, ζ_t) or (x, u, v, a, t, ζ) so that the tangent bundle projection map $\tau_P : TP \rightarrow P$ is given by $\tau_P(u_x, a_v, \zeta_t) = (x, v, t)$. Also endow P with the metric that appeared in the first part of this paper:

$$\left\langle (u_x, a_v, \zeta_t), (u'_x, a'_v, \zeta'_t) \right\rangle = u \cdot u' + a \cdot a' + \zeta \cdot \zeta'. \quad (13)$$

Let \mathbf{A} denote the magnetic vector potential vector field and $\mathbf{B} = \nabla \times \mathbf{A}$ denote the magnetic

field. Then the Poincaré-Cartan one-form, ordered in one of the standard ways², is given by

$$\begin{aligned}\vartheta_\epsilon(x, v, t) &= \mathbf{A}(x) \cdot dx + \epsilon v \cdot dx - \epsilon^2 \frac{1}{2} v \cdot v dt \\ &= \vartheta^0 + \epsilon \vartheta^1 + \epsilon^2 \vartheta^2.\end{aligned}\tag{14}$$

One can consider all variables dimensionless or not. In the latter case, \mathbf{A} should be considered to be normalized by the charge-to-mass ratio of the particle in question so that $\nabla \times \mathbf{A}$ has the units of frequency.

This one-form defines the dynamical vector field $X_\epsilon(x, v, t) = (x, \dot{x}(x, v), v, \dot{v}(x, v), t, 1)$ through the formula

$$X_\epsilon \lrcorner d\vartheta_\epsilon = 0.\tag{15}$$

It is straightforward to verify that this implies

$$\dot{x}(x, v) = \epsilon v\tag{16}$$

$$\dot{v}(x, v) = v \times \mathbf{B}(x).\tag{17}$$

The zero'th order system, which according to the previous expression is the limit of infinitely slow drift both along and across the field lines, admits the following S^1 -action $\Phi^0 : S^1 \times P \rightarrow P$ as a symmetry:

$$\Phi_\theta^0(x, v, t) = (x, \exp(-\theta \hat{b}(x)) v, t)\tag{18}$$

$$\Phi_\theta^{0*} X_0 = X_0$$

$$\Phi_\theta^{0*} d\vartheta_0 = d\vartheta_0,$$

where $b = \mathbf{B}/\|\mathbf{B}\|$. We will refer to this circle action Φ^0 as the gyrosymmetry. Note the similarity with the action on SD considered in the first part of this paper. An important difference is the “ $-$ ” in the exponential, which was chosen so that this action rotates velocity vectors in the same sense that the magnetic field rotates charged particles. It leaves $d\vartheta_0 = * \mathbf{B} \cdot dx$ invariant because \mathbf{B} is parallel to the rotation vector, and it leaves X_0 invariant because it commutes with the flow of the zero'th order system.

The action is not free, however, because those velocity vectors parallel to the magnetic field are fixed by the group action. In order to alleviate this issue, from here on we will suppose that P has those points removed that correspond to velocity vectors purely parallel

to \mathbf{B} . With this in mind, (P, Φ^0) forms a principal circle bundle. The base space P/S^1 can be identified with the space $M \equiv D \times \mathbb{R} \times \mathbb{R}^+ \times \mathbb{R}$, where $\mathbb{R}^+ = (0, \infty)$, with the bundle projection map $\pi : P \rightarrow M$ given by

$$\pi(x, v, t) = (x, b(x) \cdot v, \|(1 - b(x)b(x)) \cdot v\|, t). \quad (19)$$

Thus, the first factor of M is the physical domain, the second is parallel velocity, the third perpendicular velocity, and the fourth time. Accordingly, denote a typical element of M by $(x, v_{\parallel}, v_{\perp}, t)$. In addition, this bundle admits the principal connection $\mathcal{A}^0 : TP \rightarrow \mathbb{R}$ given by

$$\begin{aligned} \mathcal{A}^0(x, u, v, a, t, \zeta) = & \\ & - a \cdot \frac{b(x) \times v}{\|b(x) \times v\|^2} + \frac{v \cdot b(x)}{\|b(x) \times v\|} \left(u \cdot \nabla b \cdot \frac{b(x) \times v}{\|b(x) \times v\|} \right). \end{aligned} \quad (20)$$

We call this the guiding center connection. Notice that on the subset of P defined by $v \cdot b(x) = 0, \|v\| = 1$, it agrees with the connection introduced earlier on SD . As before, it is straightforward to check that this one-form satisfies the two properties in the definition of a principal connection.

Now, following Ref. 27, we would like to find a sequence of *globally defined* near-identity coordinate changes, $F^1, F^2, \dots : P \rightarrow P$, such that, in the new coordinates, the gyrosymmetry persists. We would also like each of these near-identity coordinate changes F^n to be equal to the flow map of some vector field $\epsilon^n G^n$. Thus we require that $d\hat{\vartheta} = \dots F_*^3 F_*^2 F_*^1 d\vartheta_\epsilon$ satisfy the condition $\Phi_\theta^{0*} d\hat{\vartheta} = d\hat{\vartheta}$. This implies the following well-known sequence of conditions on the G_n :

$$\begin{aligned} \Phi_\theta^{0*} \left(\vartheta^0 + \alpha^0 \right) &= \vartheta^0 + \alpha^0 \\ \Phi_\theta^{0*} \left(\vartheta^1 - L_{G^1} \vartheta^0 + \alpha^1 \right) &= \vartheta^1 - L_{G^1} \vartheta^0 + \alpha^1 \\ \dots & \end{aligned} \quad (21)$$

where the α^n comprise a sequence of undetermined closed (not necessarily exact) one-forms.

While we would like the F^n , and therefore the G^n , to be globally defined, when deriving expressions for the G^n it would be advantageous to work in the local bundle charts naturally associated to the principal circle bundle (P, Φ^0) . This is because the bundle charts put the direction of symmetry along one of the coordinate axes, thereby facilitating Fourier analysis,

as well as finding the reduced phase space²³. Fortunately, if the local expressions for G^n can be constructed subject to the conditions in appendix B, any drawback associated with doing local calculations can be avoided because these local expressions will then transform as they must. So let's examine the form of these bundle charts and the local expressions for the G^n more carefully.

First we will determine the form of a local section $s_\alpha : U_\alpha \rightarrow \pi^{-1}(U_\alpha)$, where $U_\alpha \subseteq M$. By the definition of a local section, $\pi(s_\alpha(x, v_\parallel, v_\perp, t)) = (x, v_\parallel, v_\perp, t)$. We will use this constraint to determine the general form of s_α . Set $s_\alpha(x, v_\parallel, v_\perp, t) = (X(x, v_\parallel, v_\perp, t), V(x, v_\parallel, v_\perp, t), T(x, v_\parallel, v_\perp, t))$. Note that s_α must be of this form. However, there are constraints on the component functions X, V, T . In particular, the following must be true:

$$\begin{aligned} X(x, v_\parallel, v_\perp, t) &= x & (22) \\ T(x, v_\parallel, v_\perp, t) &= t \\ V(x, v_\parallel, v_\perp, t) \cdot b(x) &= v_\parallel \\ \|(1 - b(x)b(x)) \cdot V(x, v_\parallel, v_\perp, t)\| &= v_\perp. \end{aligned}$$

To unravel these constraints, decompose $V(x, v_\parallel, v_\perp, t) = V_\parallel(x, v_\parallel, v_\perp, t)b(x) + V_\perp(x, v_\parallel, v_\perp, t)$, where $V_\perp(x, v_\parallel, v_\perp, t) = (1 - b(x)b(x)) \cdot V(x, v_\parallel, v_\perp, t)$. Then define $e_\alpha = V_\perp / \|V_\perp\|$. Employing these definitions, s_α must have the form

$$s_\alpha(x, v_\parallel, v_\perp, t) = (x, v_\parallel b(x) + v_\perp e_\alpha(x, v_\parallel, v_\perp, t), t), \quad (23)$$

where $e_\alpha(x, v_\parallel, v_\perp, t)$ must be of unit length and perpendicular to $b(x)$. See Fig. 3. We lose nothing²⁹ by making the replacement $e_\alpha(x, v_\parallel, v_\perp, t) \rightarrow e_\alpha(x)$.

Given such an s_α , the corresponding bundle chart $\phi_\alpha : \pi^{-1}(U_\alpha) \rightarrow U_\alpha \times S^1$ can be deduced (appendix A). All that must be done is find the shape of $g_\alpha : \pi^{-1}(U_\alpha) \rightarrow S^1$. If $p = (x, v, t) \in \pi^{-1}(U_\alpha)$, then by the defining relation $p = \Phi_{g_\alpha(p)}^0(s_\alpha(\pi(p)))$,

$$g_\alpha(x, v, t) = -\text{Arctan}\left(\frac{v \cdot \{b(x) \times e_\alpha(\pi(x, v, t))\}}{v \cdot e_\alpha(\pi(x, v, t))}\right). \quad (24)$$

This expression for g_α shows that the value of g_α is none other than the gyrophase measured with respect to e_α in a left-handed sense with respect to b . So it is fair to write $g_\alpha = \theta_\alpha$, with θ denoting gyrophase, and α indicating which convention, or gyrogauge is being used. Therefore the bundle charts, $\phi_\alpha(x, v, t) = (\pi(x, v, t), g_\alpha(x, v, t)) = (x, v_\parallel, v_\perp, t, \theta_\alpha)$, are none

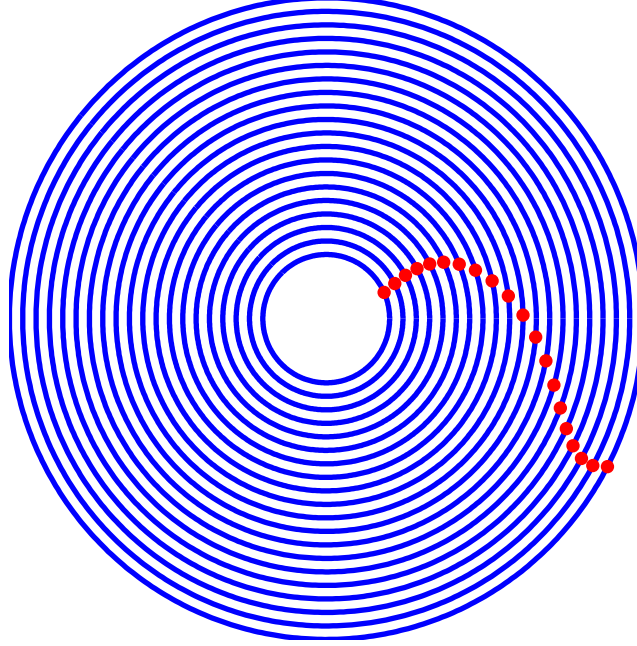


FIG. 3. A view of the $v_{\parallel} = 0$ plane of a typical velocity space $T_x D$. The Kruskal Rings appear as concentric circles from this perspective. Each ring is uniquely determined by its parameters $x, v_{\parallel}, v_{\perp}, t$ corresponding to which velocity space the ring lives in, its height along the b -axis, its radius, and its position in time, respectively. The role of e_{α} is depicted using dots; a reference point is assigned to the Kruskal Ring with parameters $x, v_{\parallel}, v_{\perp}, t$ equal to $v_{\parallel} b(x) + v_{\perp} e_{\alpha}(x, v_{\parallel}, v_{\perp}, t)$.

other than the commonly used cylindrical parameterizations of velocity space alluded to in the introduction!

Now consider the local expression for a globally defined vector field $G : P \rightarrow TP$ in one of these bundle charts. In the language used in appendix B, we are considering here $G_{\alpha}(u, \theta) = (w_{\alpha}(u, \theta), \theta, \xi_{\alpha}(u, \theta))$. Set

$$w_{\alpha} = G_M^{\alpha} = G_x^{\alpha} \cdot \frac{\partial}{\partial x} + G_{v_{\parallel}}^{\alpha} \frac{\partial}{\partial v_{\parallel}} + G_{v_{\perp}}^{\alpha} \frac{\partial}{\partial v_{\perp}} + G_t^{\alpha} \frac{\partial}{\partial t} \quad (25)$$

$$\xi_{\alpha} = G_{\theta}^{\alpha}. \quad (26)$$

These component functions must transform as described in appendix B. Thus, $G_x^{\alpha}, G_{v_{\parallel}}^{\alpha}, G_{v_{\perp}}^{\alpha}, G_t^{\alpha}$ and $\eta_{\alpha} = G_{\theta}^{\alpha} + A_{\alpha} \circ G_M^{\alpha}$ must be local representatives of globally defined quantities. These conditions are actually equivalent to those found in Ref. 30 for gyrogauged invariant Lie generators. To show this, we compute the gauge fields associated with the connection form

given earlier explicitly,

$$A_\alpha(x, v_\parallel, v_\perp, t) = - [(\nabla e_\alpha(x)) \cdot b(x) \times e_\alpha(x)] \cdot dx \quad (27)$$

So the one-form A_α is made up of Littlejohn's³⁰ R :

$$A_\alpha = -R \cdot dx, \quad (28)$$

which is exactly the gauge field that appeared while working with SD . Therefore, because G_θ^α must be the sum of the local representative of a globally defined quantity and $-A_\alpha \circ G_M^\alpha$,

$$\begin{aligned} G_\theta^\alpha &= \eta_\alpha - A_\alpha \circ G_M^\alpha \\ &= \eta_\alpha + R \cdot G_x^\alpha, \end{aligned} \quad (29)$$

which is precisely the condition in Ref. 30. This proves that

$$\text{gyrogauge invariant local Lie generators} \quad (30)$$

\Leftrightarrow

globally consistent local Lie generators.

It follows then that the existing expressions for gyrogauge invariant Lie generators, such as those given in Ref. 31, are sufficient to produce a globally consistent guiding center theory when the perpendicular unit vectors cannot be globally defined.

We need to stress here that we have *not* arrived at a new way to perform the guiding center perturbation analysis. The above analysis instead demonstrates how the concept of gyrogauge invariance appears as merely a special case of a more general mathematical theory (the theory outlined in appendix B); when looking through the lens of the theory of principal bundles, gyrogauge invariance appears naturally as a way making sure local expressions consistently define a global quantity. We also hope that illustrating this point has made it clear when the use of gyrogauge invariant generators is “mandatory”. When a perpendicular unit vector *can* be globally defined, gyrogauge invariant Lie generators are *not* required because expressions involving the perpendicular unit vectors become globally defined. This is true in spite of the fact that using gyrogauge invariant Lie generators in these cases leads to dynamical equations that are easier to interpret physically. However, when global perpendicular unit vectors fail to exist, gyrogauge invariant Lie generators provide the

only reasonable means for ensuring that the transformed equations of motion are globally defined.

To drive all of this home, we will conclude this section by demonstrating that expressions for the new Poincaré-Cartan one-form obtained using gyrogauge invariant generators can be expressed in terms of physical quantities alone. The gyrogauge invariant expression in Ref. 30 for the local representative of the Poincaré-Cartan one-form is

$$\begin{aligned} \hat{\vartheta}_\alpha(x, v_\parallel, v_\perp, t) = & \left(\mathbf{A}(x) + v_\parallel b(x) \right) \cdot dx \\ & + \frac{1}{2} \frac{v_\perp^2}{\|\mathbf{B}(x)\|} \left(d\theta - R(x) \cdot dx \right) - \left(\frac{1}{2} v_\parallel^2 + \frac{1}{2} v_\perp^2 \right) dt, \end{aligned} \quad (31)$$

which involves the unphysical e_1, e_2 through R . However, the combination $d\theta - R \cdot dx$ is actually equal to the guiding center connection expressed in the bundle chart ϕ_α (see appendix B). Therefore, upon changing back to the natural rectangular position and velocity space representation of the phase space (i.e. applying ϕ_α^* to $\hat{\vartheta}_\alpha$), the Poincaré-Cartan form becomes

$$\begin{aligned} \hat{\vartheta}(x, v, t) = & \left(\mathbf{A}(x) + v \cdot b(x) b(x) \right) \cdot dx \\ & + \frac{1}{2} \frac{(\Pi(x) \cdot v)^2}{\|\mathbf{B}(x)\|} \left[\left(\nabla b \cdot \frac{b(x) \times v v \cdot b(x)}{\|b(x) \times v\|^2} \right) \cdot dx \right. \\ & \left. - \left(\frac{b(x) \times v}{\|b(x) \times v\|^2} \right) \cdot dv \right] - \frac{1}{2} v \cdot v dt, \end{aligned} \quad (32)$$

where $\Pi(x) = 1 - b(x)b(x)$ is the perpendicular projection tensor. This one-form satisfies $\Phi_\theta^{0*} \hat{\vartheta} = \hat{\vartheta}$ *exactly* for all $\theta \in S^1$ and clearly only involves physical quantities. It also has the following geometrically appealing expression:

$$\hat{\vartheta} = \tau_D^* A + \langle \vartheta_o \rangle + \mu \mathcal{A}^0 - \frac{1}{2} \mathbf{I} dt, \quad (33)$$

where, in left-to-right order, the symbols that appear are TD 's projection map, the magnetic vector potential one-form, the averaged canonical one-form on P , the momentum map associated to the gyrosymmetry, the guiding center connection, and the first fundamental form associated to the metric on D . We would also like to point out that this result can be derived directly without ever resorting to the bundle charts³².

VI. CONCLUSION AND DISCUSSION

At last we have shown how the guiding center theory works when perpendicular unit vectors cannot be defined globally. Along the way, we identified the obstruction to the global existence of these vectors in terms of integrals of the vector N . Through examples, we showed that this obstruction does not trivially vanish in all cases. However, we demonstrated that when the physical domain particles move through is an open solid torus, it *does* vanish.

Throughout our discussion, principal circle bundles have played a central role. They at once provided the framework for our identification of the obstruction to global perpendicular unit vectors and the organizational tool that allowed us to determine how Lie perturbation theory can be done in a global way via stitching together a number of local calculations. While the mathematical theory of principal circle bundles may not be well known amongst plasma physicists, we have shown that much of the existing guiding center theory, from the time-honored cylindrical parameterization of the velocity space to the modern notion of gyro-gauge invariance, fits perfectly in this framework. But we have also seen that by recognizing the presence of this structure in the guiding center problem, and working with it directly, the guiding center Poincaré-Cartan one-form can be expressed in cartesian position and velocity space in a way that is manifestly independent of the perpendicular unit vectors.

Looking at what we have done from a practical point of view, we have identified some difficulties researchers will face when trying to simulate gyro-phase-dependent dynamics³³⁻³⁵ in configurations where global perpendicular unit vectors cannot be defined. When dealing with such deviant cases numerically, for instance in a particle-in-cell simulation, it will be necessary to either define a number of gyro-phase conventions that cover the phase space and keep track of which of these “patches” particles live in, or resort to the global expression for the Poincaré-Cartan one-form given at the end of the previous section. In the former case, care must be taken to avoid spending too much time keeping track of a particle’s “patch”, while in the latter case this could be avoided. However, the cost incurred by using the global version of the one-form comes in the form of complicated equations of motion. While simulations of the interior of tokamaks should be able to avoid multiple gyro-phase conventions by finding global perpendicular unit vectors (which must exist), this may not be the case in configurations that involve field nulls in the region of interest. These field nulls will in general put “holes” in the guiding center phase space that open up the possibility for

a lack of global perpendicular unit vectors.

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Appendix A: Principal circle bundles

Here we define and discuss the notion of principal circle bundle. A more complete exposition can be found in Ref. 36. First some terminology. Let P be a manifold and $\Phi : S^1 \times P \rightarrow P$ a smooth map, where $S^1 = \mathbb{R} \bmod 2\pi$ denotes the circle. If $\theta_1, \theta_2 \in S^1$, then we take the symbol $\theta_1 + \theta_2$ to mean addition modulo 2π . For a fixed $\theta \in S^1$ define the map $\Phi_\theta : P \rightarrow P$ by the formula $\Phi_\theta(p) = \Phi(\theta, p)$, where p is any point in P . Φ is said to be a left circle action when $\Phi_{\theta_1} \circ \Phi_{\theta_2} = \Phi_{\theta_1 + \theta_2}$ and Φ_0 is the identity on P . Given a point $p \in P$, the set $\mathcal{O}_p = \{p' \in P \mid \exists \theta \in S^1 \text{ s.t. } \Phi_\theta(p) = p'\}$ is called the orbit of Φ through p . A left circle action is said to be free if $\Phi_\theta(p) = p$ if and only if $\theta = 0$. Intuitively, a left circle action is free if when the second argument of Φ is held fixed at p_o , the resulting map establishes a one-to-one correspondence between the orbit through p_o and the circle. A *principal circle bundle* is a manifold P together with a free left circle action $\Phi : S^1 \times P \rightarrow P$. If there is a manifold B and a smooth map $\pi : P \rightarrow B$ such that π is surjective, its Jacobian matrix has full rank at each point $p \in P$, and $\pi^{-1}(b)$ is an entire orbit for each $b \in B$, then $P/S^1 \equiv B$ is referred to as the base of the principal circle bundle P and π is referred to as the bundle projection map. Because it can be shown²³ such a B and π can always be found for a principal circle bundle, the following intuitive picture of such bundles emerges. A principal circle bundle is nothing more than a collection of circles (the orbits) smoothly parameterized by the base P/S^1 .

There is a subtle aspect of this picture however. Notice that while it is possible to fix a point $p_o \in P$ as the second argument in Φ and establish a correspondence between the orbit through p_o and S^1 , if $\Phi_\theta(p_o)$ were used in place of p_o , the result would be a *different* correspondence between the same two objects \mathcal{O}_{p_o} and S^1 . This is because $\mathcal{O}_{p_o} = \mathcal{O}_{\Phi_\theta(p_o)}$. Therefore, while the orbits \mathcal{O}_p “look” like distorted copies of the circle, they lack a natural

choice for the 0, or reference angle.

On the other hand, it is often convenient take a bunch of nearby orbits and smoothly assign to each of them a reference point so that each point on this bunch of orbits can be assigned an angle in an unambiguous way. Such an assignment of reference points is called a local section. Formally, given an open subset $U_\alpha \subset P/S^1$ of the base, a local section $s_\alpha : U_\alpha \rightarrow \pi^{-1}(U_\alpha)$ is a mapping from U_α into the collection of orbits that project onto U_α that satisfies the equation $\pi \circ s_\alpha = \text{id}_{U_\alpha}$, which simply says that s_α assigns a single point to each of the orbits “attached” to U_α . Local sections can always be found. However, a global section $s : P/S^1 \rightarrow P$, which would smoothly assign a reference point to *all* of the orbits that make up P , may not exist. If a global section does exist, then the principal bundle is referred to as being *trivial*.

In the presence of a local section, the process of assigning an angle to each point in the bunch of orbits attached to U_α can be formalized as a special coordinate system on $\pi^{-1}(U_\alpha)$ known as a bundle chart. If $p \in \pi^{-1}(U_\alpha)$, then, because the action is free, there is a unique $g_\alpha(p) \in S^1$ such that $p = \Phi_{g_\alpha(p)} s_\alpha(\pi(p))$. This defines the functions $g_\alpha : \pi^{-1}(U_\alpha) \rightarrow S^1$. The bundle charts $\phi_\alpha : \pi^{-1}(U_\alpha) \rightarrow U_\alpha \times S^1$ are then given by the formula $\phi_\alpha(p) = (\pi(p), g_\alpha(p))$. By this definition, when looking at a principal circle bundle locally in a bundle chart, it looks like a bunch of bike tires hanging on a multi-dimensional horizontal rod. The orbits are the tires while the base is the rod. It is also useful to think of the bundle charts as “symmetry-aligned” coordinate systems, where the symmetry is defined by Φ .

Appendix B: Principal connections

This appendix gives the definition of a principal connection and briefly explores some of the basic properties of these objects relevant to this article. A much more thorough discussion can be found in Ref. 37.

Given a principal circle bundle (P, Φ) and a real number ξ , the *infinitesimal generator* ξ_P associated to ξ is the vector field on P given by $\xi_P(p) = \left. \frac{d}{d\theta} \right|_{\theta=0} \Phi_{\xi\theta}(p)$. So ξ_P points in the direction of the symmetry associated with Φ . A *principal connection*, or connection form on

P is a one-form, \mathcal{A} , with the following two properties:

- 1) $\forall \xi \in \mathbb{R}, \quad \mathcal{A}(\xi_P) = \xi$
- 2) $\forall \theta \in S^1, \quad \Phi_\theta^* \mathcal{A} = \mathcal{A}.$

Connection forms have a useful local structure when viewed in the bundle charts defined in the previous section. Let $s_\alpha : U_\alpha \rightarrow \pi^{-1}(U_\alpha)$ be a local section and ϕ_α its associated bundle chart. Define the gauge field $A_\alpha : T(P/S^1) \rightarrow \mathbb{R}$ and the Maurer-Cartan one-form $\theta_L : TS^1 \rightarrow \mathbb{R}$ by

$$A_\alpha = s_\alpha^* \mathcal{A} \tag{B1}$$

$$\theta_L(\theta, \xi) = \xi, \tag{B2}$$

where we have made the identification $TS^1 = S^1 \times \mathbb{R}$. Note that θ_L is nothing more than the coordinate differential on S^1 . It is not difficult to show that on $\pi^{-1}(U_\alpha)$ \mathcal{A} is made up of these two quantities according to

$$\mathcal{A} = \pi^* A_\alpha + g_\alpha^* \theta_L. \tag{B3}$$

This formula has two important consequences. First of all, if A_β is another gauge field defined on an overlapping patch of P/S^1 , $U_\alpha \cap U_\beta \neq \emptyset$, then it must be related to A_α on the overlap:

$$A_\alpha = A_\beta + g_{\alpha\beta}^* \theta_L, \tag{B4}$$

where $g_{\alpha\beta} : U_\alpha \cap U_\beta \rightarrow S^1$ is the circle-valued function defined by the relation $g_{\alpha\beta}(\pi(p)) = g_\beta(p) - g_\alpha(p)$. Second, it implies that the *gauge field strengths* $F_\alpha = dA_\alpha$, apparently only locally defined quantities, actually define a global two-form, the *curvature form* F , over the entire base P/S^1 . This result follows from applying the exterior derivative to (B4) and recalling that $d\theta_L = 0$. On any of the U_α , $F = F_\alpha$. As discussed in Ref. 24, the curvature two-form encodes the basic topological properties of the principal circle bundle it comes from.

Connection forms also provide a convenient structure for expressing the transformation law for the bundle chart representatives of globally defined vector fields on P . If $X : P \rightarrow TP$ is a smooth vector field on P , then given a bundle chart ϕ_α , its bundle chart representative is $X_\alpha \equiv \phi_{\alpha*} X : U_\alpha \times S^1 \rightarrow TU_\alpha \times S^1 \times \mathbb{R}$; the bundle chart representatives

are just the vector field expressed in the coordinates provided by the bundle charts. Set $X_\alpha(u, \theta) = (w_\alpha(u, \theta), \theta, \xi_\alpha(u, \theta))$, where $w_\alpha(u, \theta) \in T_u(P/S^1)$ and $\xi_\alpha(u, \theta) \in \mathbb{R}$. Using the fact that $\phi_\alpha^* X_\alpha = \phi_\beta^* X_\beta$ on $\pi^{-1}(U_\alpha \cap U_\beta)$, it is straightforward to show that the bundle chart representatives are related by

$$w_\alpha(u, \theta) = w_\beta(u, \theta') \tag{B5}$$

$$\xi_\alpha(u, \theta) = \xi_\beta(u, \theta') + g_{\beta\alpha}^* \theta_L(w_\beta(u, \theta')), \tag{B6}$$

where $\theta' = \theta + g_{\alpha\beta}(u)$. Using the transformation law for the gauge fields, this can be recast as

$$\eta_\alpha(u, \theta) \equiv \xi_\alpha(u, \theta) + A_\alpha(w_\alpha(u, \theta)) \tag{B7}$$

$$w_\alpha(u, \theta) = w_\beta(u, \theta') \tag{B8}$$

$$\eta_\alpha(u, \theta) = \eta_\beta(u, \theta'). \tag{B9}$$

So we see that the w_α and η_α are local representatives of globally defined maps. To be precise, $w_\alpha = w \circ \phi_\alpha^{-1}$ and $\eta_\alpha = \eta \circ \phi_\alpha^{-1}$, where $w : P \rightarrow T(P/S^1)$ and $\eta : P \rightarrow \mathbb{R}$ are globally defined maps only constrained to satisfy $\tau_{P/S^1} \circ w = \pi$ (τ_{P/S^1} is the tangent bundle projection map associated to $T(P/S^1)$).

Conversely, if there is an assignment of a local vector field X_α to each of the bundle charts ϕ_α whose components satisfy (B8) and (B9), then this collection of locally defined vector fields will define a global vector field $X : P \rightarrow TP$ that agrees with each of the X_α in the bundle charts.

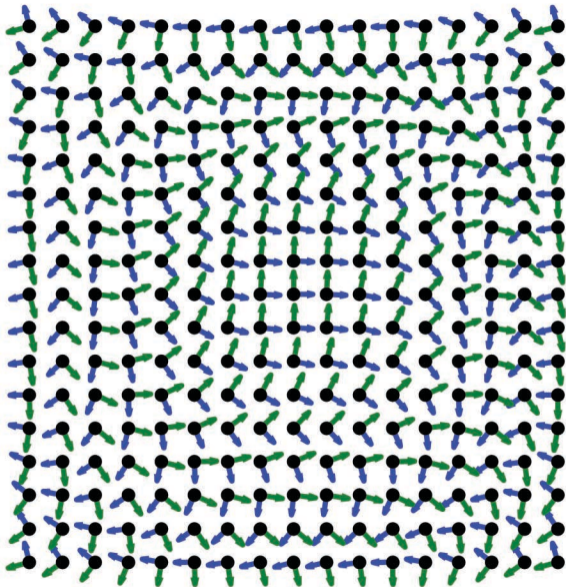
Why is expressing the vector transformation law in terms of the gauge fields useful? Because of the organization it brings to the process of stitching together local vector fields into a global one. The vector transformation law for passing from one arbitrary (non-bundle) coordinate chart to another would be quite messy to work with for this purpose. By working with the bundle charts and finding expressions for the gauge fields, the process is streamlined to finding the two functions w and η .

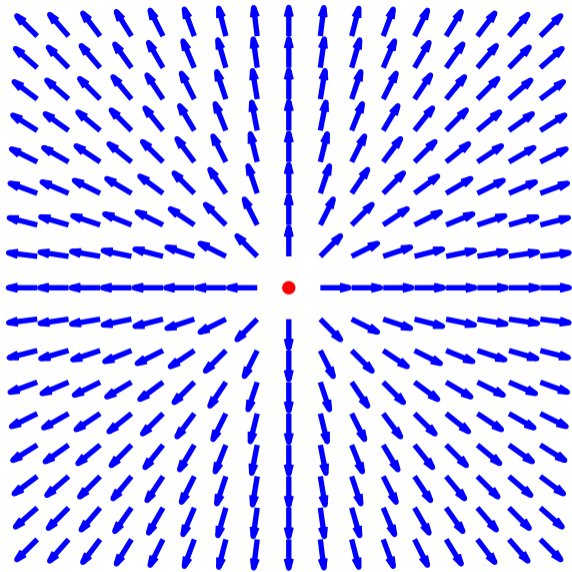
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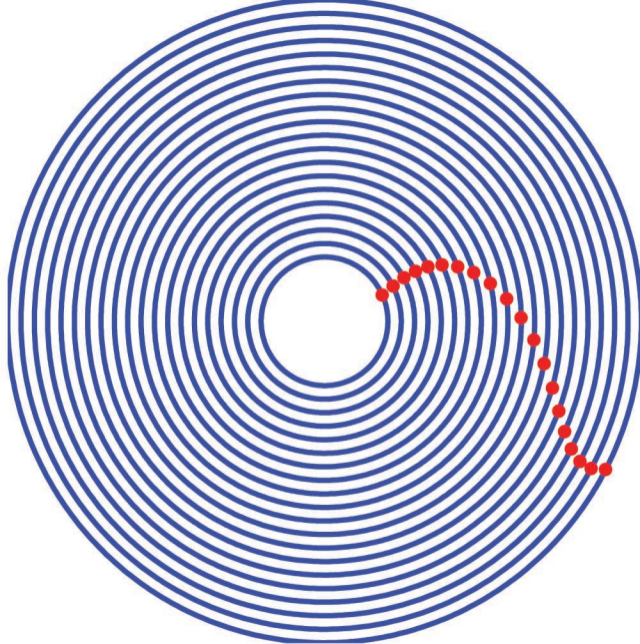
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