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Lagrangian and Hamiltonian constraints for guiding-center Hamiltonian theories

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A consistent guiding-center Hamiltonian theory is derived by Lie-transform perturbation method, with terms up to second order in magnetic-field nonuniformity. Consistency is demonstrated by showing that the guiding-center transformation presented here satisfies separate Jacobian and Lagrangian constraints that have not been explored before. A new first-order term appearing in the guiding-center phase-space Lagrangian is identified through a calculation of the guiding-center polarization. It is shown that this new polarization term also yields a simpler expression of the guiding-center toroidal canonical momentum, which satisfies an exact conservation law in axisymmetric magnetic geometries. Lastly, an application of the guiding-center Lagrangian constraint on the guiding-center Hamiltonian yields a natural interpretation for its higher-order corrections.

I. INTRODUCTION

The consistent derivation of a Hamiltonian guiding-center theory that includes second-order effects in magnetic-field nonuniformity is an important problem in magnetic fusion plasma physics. While the derivation of the second-order corrections in the guiding-center Hamiltonian equations of motion yield higher-order corrections that may be ignored in practical applications, they can nonetheless be useful in gaining insights into higher-order perturbation theory.

A. Previous works

Recently, Parra and Calvo [1] and Burby, Squire, and Qin [2] derived guiding-center theories with second-order corrections in the guiding-center Hamiltonian using different methods. Parra and Calvo [1] constructed their guiding-center transformation based on a *microscopic* view that treats the lowest-order gyroradius $\rho_{\rm g}$ as a zeroth-order (nonperturbative) term that is introduced by a preliminary transformation, which introduces explicit gyroangle dependence in the preliminary phase-space Lagrangian. The subsequent derivation of the guiding-center phase-space Lagrangian proceeds through an asymptotic expansion in powers of a small ordering parameter $\epsilon_{\rm B} \equiv \rho_{\rm g}/L_{\rm B} \ll 1$ defined as the ratio of the gyroradius $\rho_{\rm g}$ (which is considered finite in the microscopic view) to the magnetic nonuniformity length scale $L_{\rm B} \gg \rho_{\rm g}$. Burby, Squire, and Qin [2], on the other hand, derived the second-order guiding-center Hamiltonian through a computer-based algorithm that bypassed the issue of gyrogauge invariance.

These two theories were compared in Ref. [3] and were found to agree up to a gyroangle-independent gauge term in the guiding-center phase-space Lagrangian. Both works reproduced the first-order results of the pioneering work of Littlejohn [4–6], which made certain simplifying assumptions on the symplectic part of the guiding-center phase-space Lagrangian (see Ref. [7] for a review).

B. Present work

The purpose of the present work is to use the standard Lie-transform perturbation method to derive higher-order guiding-center Hamilton equations of motion with as few assumptions about the guiding-center Hamiltonian and Poisson-bracket structure as possible. The consistency of our guiding-center transformation is checked through Jacobian, Hamiltonian, and Lagrangian constraints.

In the process, we show that a consistent treatment of guiding-center polarization [8, 9] and a more transparent guiding-center representation of the toroidal canonical angular momentum, which is an exact constant of motion in axisymmetric magnetic geometry, both require that a new first-order term be kept in the symplectic part of the guiding-center phase-space Lagrangian [10].

C. Organization

The remainder of the paper is organized as follows. In Sec. II, equivalent representations of guiding-center Hamiltonian theory are presented in terms of the guiding-center Hamiltonian (1) and the guiding-center Poisson bracket (10), in which the guiding-center magnetic moment $\mu \equiv J\,\Omega/B$ (expressed in terms of the gyroaction J) is uniquely defined and higher-order corrections due to magnetic-field nonuniformity are included in either the guiding-center potential energy $\Psi \equiv J\,\Omega + \cdots$ or the guiding-center symplectic momentum $\mathbf{\Pi} \equiv p_{\|}\,\widehat{\sf b} + \cdots$. In the Hamiltonian representation ($\mathbf{\Pi} \equiv p_{\|}\widehat{\sf b}$), these higher-order corrections appear only in the guiding-center Hamiltonian, while, in the symplectic representation ($\Psi \equiv J\,\Omega$), they appear only in the guiding-center Poisson bracket.

In Sec. III, the higher-order guiding-center transformation is given up to second order in magnetic-field nonuniformity, and it is shown to simultaneously satisfy several consistency constraints based on the guiding-center Jacobian, Hamiltonian, and Lagrangian. These constraints leave only the perpendicular components of the first-order symplectic momentum $\mathbf{\Pi}_{1\perp}$ unspecified. In previous works, from Littlejohn's work [4–6] up until recent work [1, 2], the choice $\mathbf{\Pi}_{1\perp} \equiv 0$ was implicitly assumed. In Ref. [10], it was shown that a new constraint on the choice for $\mathbf{\Pi}_{1\perp}$ is imposed if the guiding-center transformation introduced in Sec. III is to yield the standard Pfirsch-Kaufman expression for the guiding-center polarization [8, 9]. This new choice is shown in Sec. IV to lead to a more transparent guiding-center representation for the toroidal canonical momentum, which is an exact constant of motion in axisymmetric tokamak geometry.

II. HIGHER-ORDER GUIDING-CENTER HAMILTONIAN THEORY

In the perturbation analysis that follows, we use the *macroscopic* view (i.e., $L_{\rm B}$ is finite and $\rho_{\rm g} \ll L_{\rm B}$), which is implemented through the ordering parameter ϵ introduced by renormalizing the electric charge $e \to e/\epsilon$ (e.g., $\Omega = eB/mc \to \epsilon^{-1}\Omega$) [7]. According to this view, a preliminary phase-space transformation is not required and physical results are recovered by setting $\epsilon = 1$.

A. Guiding-center Hamiltonian and Poisson-bracket structure

Guiding-center Hamiltonian dynamics is expressed in terms of a guiding-center Hamiltonian function that depends on the guiding-center position $\mathbf{X}$, the guiding-center parallel momentum $p_\parallel$, and the guiding-center gyroaction $J \equiv \mu\, B/\Omega$; it is, however, independent of the gyroangle θ at all orders. Since the guiding-center phase-space coordinates are non-canonical coordinates, a non-canonical guiding-center Poisson bracket is also needed.

1. *Equivalent Hamiltonian theories*

In the present work, the guiding-center Hamiltonian is defined as

$$H_{\rm gc} \;\equiv\; \frac{p_\parallel^2}{2m} \;+\; \Psi, \tag{1}$$

where the effective guiding-center potential energy

$$\Psi \;\equiv\; J\,\Omega \;+\; \epsilon\,\Psi_1 \;+\; \epsilon^2\,\Psi_2 \;+\; \cdots \tag{2}$$

is defined in terms of the gyroangle-independent scalar fields Ψ_n ($n \geq 1$), which contain corrections due to magnetic-field nonuniformity.

The guiding-center symplectic structure is expressed in terms of the guiding-center Poincaré-Cartan one-form

$$\Gamma_{\rm gc} \;\equiv\; \left(\frac{e}{\epsilon c}\mathbf{A} \;+\; \mathbf{\Pi}\right)\boldsymbol{\cdot}\,\mathsf{d}\mathbf{X} \;+\; \epsilon\,J\,(\mathsf{d}\theta \;-\; \mathbf{R}\boldsymbol{\cdot}\mathsf{d}\mathbf{X}), \tag{3}$$

where the symplectic guiding-center momentum

$$\mathbf{\Pi} \;\equiv\; \sum_{n=0}^{\infty}\epsilon^n\,\mathbf{\Pi}_n \;=\; p_\parallel\,\widehat{\mathsf{b}} \;+\; \epsilon\,\mathbf{\Pi}_1 \;+\; \epsilon^2\,\mathbf{\Pi}_2 + \cdots \tag{4}$$

is expressed in terms of the gyroangle-independent vector fields $\mathbf{\Pi}_n$ ($n \geq 1$), which contain corrections due to magnetic-field nonuniformity. The presence of the gyrogauge vector $\mathbf{R}$ guarantees that the the guiding-center one-form (3) is gyrogauge-invariant [6].

Guiding-center theories are said to be *equivalent* [11] if they have the same definition of the guiding-center gyroaction J but different definitions of the scalar field Ψ and the vector field $\mathbf{\Pi}$. This equivalence class will be expressed at each order in terms of a relation involving the combination $\Psi_n - \Pi_{n\parallel}\; p_\parallel/m$, where $\Pi_{n\parallel} \;\equiv\; \widehat{\mathsf{b}}\boldsymbol{\cdot}\mathbf{\Pi}_n$ denotes the parallel component of $\mathbf{\Pi}_n$.

In a purely *Hamiltonian* representation ($\mathbf{\Pi}_n \equiv 0,\; n \geq 1$), the vector field $\mathbf{\Pi} \equiv p_\parallel\,\widehat{\mathsf{b}}$ is independent of the gyroaction J, while the scalar field $\Psi \equiv J\,\Omega + \epsilon\,\Psi_1 + \epsilon^2\,\Psi_2 + \cdots$ contains all the correction terms associated with the nonuniformity of the magnetic field. In a purely *symplectic* representation ($\Psi_n \equiv 0,\; n \geq 1$), on the other hand, the scalar field $\Psi \equiv J\,\Omega$ is independent of the parallel momentum $p_\parallel$, while the vector field $\mathbf{\Pi} = p_\parallel\,\widehat{\mathsf{b}} + \epsilon\,\mathbf{\Pi}_1 + \cdots$ contains all the correction terms associated with the nonuniformity of the magnetic field. Our analysis shows that, while a purely Hamiltonian representation is possible at all orders, a purely symplectic representation is possible only at first order. We note that previous guiding-center Hamiltonian theories were constructed in a mixed representation.

2. *Guiding-center Poisson bracket*

The guiding-center Poisson bracket obtained from the guiding-center Euler-Poincaré one-form (3) by following the following inversion procedure. First, we construct the guiding-center Lagrange two-form $\boldsymbol{\omega}_{\rm gc} \equiv \mathsf{d}\Gamma_{\rm gc}$. We note that the Lagrange component-matrix is invertible since the guiding-center Jacobian

$$\mathcal{J}_{\rm gc} \;\equiv\; \sqrt{\det(\boldsymbol{\omega}_{\rm gc})} \;=\; \epsilon\;\widehat{\mathsf{b}}^*\boldsymbol{\cdot}\left(\frac{e}{\epsilon\,c}\;\mathbf{B}^*\right) \;\equiv\; \frac{e}{c}\;B_\parallel^{**} \;\neq\; 0, \tag{5}$$

where we use the following definitions

$$\mathbf{B}^{*} \;\equiv\; \nabla\times\left[\mathbf{A} \,+\, \frac{c}{e}\left(\epsilon\,\boldsymbol{\Pi} \,-\, \epsilon^{2}\,J\,\mathbf{R}\right)\right], \tag{6}$$

$$\widehat{\mathsf{b}}^{*} \;\equiv\; \frac{\partial\boldsymbol{\Pi}}{\partial p_{\|}} \;=\; \widehat{\mathsf{b}} \,+\, \epsilon\,\frac{\partial\boldsymbol{\Pi}_{1}}{\partial p_{\|}} \,+\, \cdots, \tag{7}$$

$$\mathbf{R}^{*} \;\equiv\; \mathbf{R} \,-\, \epsilon^{-1}\,\frac{\partial\boldsymbol{\Pi}}{\partial J} \;=\; \mathbf{R} \,-\, \frac{\partial\boldsymbol{\Pi}_{1}}{\partial J} \,+\, \cdots, \tag{8}$$

$$B_{\|}^{**} \;\equiv\; \widehat{\mathsf{b}}^{*}\cdot\mathbf{B}^{*} = \left(\widehat{\mathsf{b}} + \epsilon\frac{\partial\boldsymbol{\Pi}_{1}}{\partial p_{\|}} + \cdots\right)\cdot\mathbf{B}^{*}. \tag{9}$$

Here, the fields $\mathbf{B}^{*}$ and $\widehat{\mathsf{b}}^{*}$ satisfy the identities $\nabla\cdot\mathbf{B}^{*} \equiv 0$, $\partial\mathbf{B}^{*}/\partial p_{\|} \equiv \epsilon\,(c/e)\,\nabla\times\widehat{\mathsf{b}}^{*}$, and $\partial\mathbf{B}^{*}/\partial J \equiv -\,\epsilon^{2}(c/e)\,\nabla\times\mathbf{R}^{*}$, which play an important role in the properties of the guiding-center Poisson bracket.

Next, we invert the guiding-center Lagrange matrix $\boldsymbol{\omega}_{\rm gc}$ to construct the guiding-center Poisson matrix with components $J_{\rm gc}^{\alpha\beta}$, such that $J_{\rm gc}^{\alpha\nu}\,\omega_{{\rm gc}\nu\beta} \equiv \delta^{\alpha}_{\beta}$. Lastly, we construct the guiding-center Poisson bracket $\{F,\,G\}_{\rm gc} \equiv (\partial F/\partial Z^{\alpha})\,J_{\rm gc}^{\alpha\beta}\,(\partial G/\partial Z^{\beta})$:

$$\begin{aligned}\Big\{F,\,G\Big\}_{\rm gc} \;=\;& \epsilon^{-1}\left(\frac{\partial F}{\partial\theta}\,\frac{\partial G}{\partial J} \,-\, \frac{\partial F}{\partial J}\,\frac{\partial G}{\partial\theta}\right) \\ &+\, \frac{\mathbf{B}^{*}}{B_{\|}^{**}}\cdot\left(\nabla^{*}F\,\frac{\partial G}{\partial p_{\|}} \,-\, \frac{\partial F}{\partial p_{\|}}\,\nabla^{*}G\right) \\ &-\, \frac{\epsilon\,c\widehat{\mathsf{b}}^{*}}{e\,B_{\|}^{**}}\cdot\nabla^{*}F\times\nabla^{*}G,\end{aligned} \tag{10}$$

where the modified gradient operator $\nabla^{*} \equiv \nabla + \mathbf{R}^{*}\partial/\partial\theta$ ensures gyrogauge-invariance. The derivation procedure of the guiding-center Poisson bracket (10) guarantees that it satisfies the standard Poisson-bracket properties, while the guiding-center Jacobian (5) can be used to write Eq. (10) in phase-space divergence form

$$\Big\{F,\,G\Big\}_{\rm gc} \;=\; \frac{1}{\mathcal{J}_{\rm gc}}\,\frac{\partial}{\partial Z^{\alpha}}\left(\mathcal{J}_{\rm gc}\,F\,\{Z^{\alpha},\,G\}_{\rm gc}\right). \tag{11}$$

B. Guiding-center Hamilton equations of motion

The Hamiltonian guiding-center equations of motion $d_{\rm gc}Z^{\alpha}/dt \equiv \{Z^{\alpha},\,H_{\rm gc}\}_{\rm gc}$ are expressed in terms of the guiding-center Hamiltonian (1) and the guiding-center Poisson bracket (10) as

$$\frac{d_{\rm gc}\mathbf{X}}{dt} \;=\; \left(\frac{p_{\|}}{m} + \frac{\partial\Psi}{\partial p_{\|}}\right)\frac{\mathbf{B}^{*}}{B_{\|}^{**}} \,+\, \frac{\epsilon\,c\widehat{\mathsf{b}}^{*}}{e\,B_{\|}^{**}}\times\nabla\Psi, \tag{12}$$

$$\frac{d_{\rm gc}p_{\|}}{dt} \;=\; -\,\frac{\mathbf{B}^{*}}{B_{\|}^{**}}\cdot\nabla\Psi, \tag{13}$$

$$\frac{d_{\rm gc}\theta}{dt} \;=\; \epsilon^{-1}\,\frac{\partial\Psi}{\partial J} \,+\, \frac{d_{\rm gc}\mathbf{X}}{dt}\cdot\mathbf{R}^{*}, \tag{14}$$

and

$$\frac{d_{\rm gc}J}{dt} \;=\; -\,\epsilon^{-1}\,\frac{\partial\Psi}{\partial\theta} \;\equiv\; 0, \tag{15}$$

where the last equation follows from the effective guiding-center potential energy Ψ being gyroangle-independent to all orders in ϵ. We note that the Hamiltonian guiding-center equations of motion (12)-(13) satisfy the guiding-center Liouville theorem

$$\nabla\cdot\left(B_{\|}^{**}\,\frac{d_{\rm gc}\mathbf{X}}{dt}\right) \,+\, \frac{\partial}{\partial p_{\|}}\left(B_{\|}^{**}\,\frac{d_{\rm gc}p_{\|}}{dt}\right) \;=\; 0, \tag{16}$$

which shows that the gyromotion action-angle dynamics, represented by Eqs. (14)-(15), is completely decoupled from the reduced guiding-center dynamics represented by Eqs. (12)-(13).

In the guiding-center Hamilton equations (12)-(15), the scalar field Ψ appears explicitly, while the symplectic momentum vector field $\boldsymbol{\Pi}$ appears implicitly in the guiding-center Poisson bracket through $\mathbf{B}^{*}$, $\widehat{\mathsf{b}}^{*}$, and $\mathbf{R}^{*}$. The advantage of the Hamiltonian representation is that the guiding-center Poisson bracket is simplified by the choice $\boldsymbol{\Pi} = p_{\|}\,\widehat{\mathsf{b}}$, while the advantage of the symplectic representation is that the guiding-center Hamiltonian is simplified by the choice $\Psi = J\,\Omega$.

III. CONSISTENT GUIDING-CENTER TRANSFORMATION

The derivation of the guiding-center Hamiltonian (1) and the guiding-center phase-space Lagrangian (3) by Lie-transform phase-space Lagrangian perturbation method is based on a phase-space transformation to guiding-center coordinates $Z^{\alpha} = (\mathbf{X}, p_{\|}; J, \theta)$ generated by the vector fields $(\mathsf{G}_{1}, \mathsf{G}_{2}, \cdots)$:

$$Z^{\alpha} \;=\; z^{\alpha} + \epsilon\,G_{1}^{\alpha} + \epsilon^{2}\left(G_{2}^{\alpha} + \frac{1}{2}\,\mathsf{G}_{1}\cdot\mathsf{d}G_{1}^{\alpha}\right) + \cdots, \tag{17}$$

with its inverse defined as

$$z^{\alpha} \;=\; Z^{\alpha} - \epsilon\,G_{1}^{\alpha} - \epsilon^{2}\left(G_{2}^{\alpha} - \frac{1}{2}\,\mathsf{G}_{1}\cdot\mathsf{d}G_{1}^{\alpha}\right) + \cdots. \tag{18}$$

While the derivation of the guiding-center phase-space coordinates may seem to allow some freedom (e.g., choosing a Hamiltonian or a symplectic representation), we must ensure that these coordinates are chosen consistently. For this purpose, a set of constraints is introduced to verify consistency at each order.

A. Guiding-center Jacobian constraints

The guiding-center Jacobian (5) associated with the phase-space transformation (17) is defined as

$$\begin{aligned}\mathcal{J}_{\rm gc} \;=\;& \mathcal{J}_{0} \,-\, \frac{\partial}{\partial Z^{\alpha}}\Big[\mathcal{J}_{0}\,\left(\epsilon\,G_{1}^{\alpha} \,+\, \epsilon^{2}\,G_{2}^{\alpha} + \cdots\right) \\ &-\, \frac{\epsilon^{2}}{2}\,G_{1}^{\alpha}\,\frac{\partial}{\partial Z^{\beta}}\left(\mathcal{J}_{0}\,G_{1}^{\beta} + \cdots\right) \,+\, \cdots\Big] \\ \equiv\;& \mathcal{J}_{0} \,+\, \epsilon\,\mathcal{J}_{1} \,+\, \epsilon^{2}\,\mathcal{J}_{2} \,+\, \cdots\end{aligned} \tag{19}$$

where $\mathcal{J}_0 \equiv e\,B/c$.

Hence, at first and second orders, the components of the first and second order generating vector fields G_1 and G_2 must satisfy the Jacobian constraints:

$$\frac{\mathcal{J}_1}{\mathcal{J}_0} \;=\; \frac{\partial\Pi_{1\|}}{\partial p_\|} \;+\; \varrho_\|\,\tau \;\equiv\; -\,\frac{1}{\mathcal{J}_0}\frac{\partial}{\partial Z^\alpha}\left(\mathcal{J}_0\,G_1^\alpha\right), \tag{20}$$

$$\begin{aligned}\frac{\mathcal{J}_2}{\mathcal{J}_0} \;&=\; \frac{\partial\Pi_{2\|}}{\partial p_\|} + \varrho_\|\,\frac{\partial\mathbf{\Pi}_1}{\partial p_\|}\cdot\nabla\times\widehat{\mathsf{b}} + \frac{c\widehat{\mathsf{b}}}{eB}\cdot\nabla\times\left(\mathbf{\Pi}_1 - J\,\mathbf{R}\right) \\ &\equiv\; -\,\frac{1}{\mathcal{J}_0}\frac{\partial}{\partial Z^\alpha}\left(\mathcal{J}_0\,G_2^\alpha \;+\; \frac{1}{2}\,\mathcal{J}_1\,G_1^\alpha\right),\end{aligned} \tag{21}$$

where $\varrho_\| \equiv p_\|/(m\Omega)$ and $\tau \equiv \widehat{\mathsf{b}}\cdot\nabla\times\widehat{\mathsf{b}}$.

We shall see below that the main result of the Jacobian constraints is that the first-order symplectic momentum must satisfy the constraint

$$\partial\mathbf{\Pi}_1/\partial p_\| \;\equiv\; 0, \tag{22}$$

which implies that $\widehat{\mathsf{b}}^* \equiv \widehat{\mathsf{b}} + \mathcal{O}(\epsilon^2)$ in Eq. (7).

B. Guiding-center Hamiltonian constraints

Another requirement for the guiding-center transformation (17) is that the definition of the guiding-center gyroaction J must be unique, which leads to the following guiding-center Hamiltonian constraints.

1. First-order Hamiltonian constraint

The second-order (ϵ^2) Lie-transform perturbation analysis yields the first-order ($\epsilon_{\rm B}$) guiding-center Hamiltonian constraint

$$\begin{aligned}\Psi_1 \;-\; \frac{p_\|}{m}\,\Pi_{1\|} \;&\equiv\; -\,\Omega\,\langle G_1^J\rangle \;-\; \frac{1}{2}\,J\,\Omega\;\varrho_\|\,\tau \\ &=\; \frac{1}{2}\,J\,\Omega\;\varrho_\|\,\tau,\end{aligned} \tag{23}$$

where $\langle G_1^J\rangle \equiv -\,J\;\varrho_\|\,\tau$ is calculated at order ϵ^3 in the Lie-transform perturbation analysis. This first-order Hamiltonian constraint, of course, has an infinite number of solutions for $(\Pi_{1\|},\Psi_1)$. One possible choice for $(\Pi_{1\|},\Psi_1)$, for example, is $\Pi_{1\|} = \frac{1}{2}\,J\,\tau$ and $\Psi_1 = J\,\Omega\;(\varrho_\|\tau)$, which allows the Baños parallel drift velocity $\partial\Psi_1/\partial p_\| = J\,\tau/m$ to be included in Eq. (12).

Here, we note that, since the right side of Eq. (23) is linear in $p_\|$, we may choose $\Psi_1 \equiv 0$ without making $\Pi_{1\|}$ singular. In accordance with standard guiding-center and gyrocenter Hamiltonian theories [7, 12], we therefore choose the first-order symplectic representation

$$\left.\begin{aligned}\Psi_1 \;&\equiv\; 0 \\ \Pi_{1\|} \;&\equiv\; -\,\tfrac{1}{2}\,J\,\tau\end{aligned}\right\}, \tag{24}$$

which satisfies the Jacobian constraint (22). We note, however, that the perpendicular component $\mathbf{\Pi}_{1\perp}$ is not constrained by the first-order Hamiltonian constraint (23).

2. Second-order Hamiltonian constraint

The third-order (ϵ^3) Lie-transform perturbation analysis yields the second-order ($\epsilon_{\rm B}^2$) guiding-center Hamiltonian constraint

$$\begin{aligned}\Psi_2 \;-\; \frac{p_\|}{m}\,\Pi_{2\|} \;\equiv\; -\,\Omega\,\langle G_2^J\rangle \;+\; J\Omega\;\varrho_\|^2\left(\frac{1}{2}\,\tau^2 - \langle\alpha_1^2\rangle\right) \\ +\;\mathbf{\Pi}_1\cdot\mathbf{v}_{\rm gc} \;-\; \frac{m}{2}\,|\mathbf{v}_{\rm gc}|^2,\end{aligned} \tag{25}$$

where $\langle G_2^J\rangle$ needs to be calculated at order ϵ^4 in the Lie-transform perturbation analysis, $\alpha_1 \equiv -\,\frac{1}{2}(\widehat{\perp}\widehat{\rho}+\widehat{\rho}\widehat{\perp}) : \nabla\widehat{\mathsf{b}}$ (where we use the rotating unit-vector basis $\widehat{\perp}\times\widehat{\rho} = \widehat{\mathsf{b}}$, with $\widehat{\perp} \equiv \partial\widehat{\rho}/\partial\theta$), and $\mathbf{v}_{\rm gc}$ denotes the lowest-order guiding-center (perpendicular) drift velocity

$$\mathbf{v}_{\rm gc} \;\equiv\; \frac{\widehat{\mathsf{b}}}{m\Omega}\times\left(J\,\nabla\Omega \;+\; \frac{p_\|^2}{m}\,\boldsymbol{\kappa}\right), \tag{26}$$

where $\boldsymbol{\kappa} \equiv \widehat{\mathsf{b}}\cdot\nabla\widehat{\mathsf{b}}$ denotes the magnetic curvature. We now see that the perpendicular component $\mathbf{\Pi}_{1\perp}$ makes its appearance in Eq. (25).

When $\langle G_2^J\rangle$ is calculated at order ϵ^4 in the Lie-transform perturbation analysis, we find

$$\langle G_2^J\rangle \;=\; \frac{J^2}{2m\Omega}\left[\frac{\tau^2}{2} + \widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} - \langle\alpha_1^2\rangle - \frac{\widehat{\mathsf{b}}}{2}\cdot\nabla\times\left(\widehat{\mathsf{b}}\times\nabla\ln B\right)\right] \;-\; \frac{J}{2}\,\varrho_\|^2\left[\boldsymbol{\kappa}\cdot\left(3\,\boldsymbol{\kappa} - \nabla\ln B\right) \;+\; \nabla\cdot\boldsymbol{\kappa} - \tau^2\right]. \tag{27}$$

which, when inserted into Eq. (25), yields the second-order ($\epsilon_{\rm B}^2$) guiding-center Hamiltonian constraint

$$\begin{aligned}\Psi_2 \;-\; \frac{p_\|}{m}\,\Pi_{2\|} \;\equiv\; J\,\Omega\left(\frac{J}{2\,m\Omega}\,\beta_{2\perp} \;+\; \frac{1}{2}\,\varrho_\|^2\,\beta_{2\|}\right) \\ -\;\frac{p_\|^2}{2m}\,\left(\varrho_\|^2\,|\boldsymbol{\kappa}|^2\right) \;+\; \mathbf{\Pi}_1\cdot\mathbf{v}_{\rm gc},\end{aligned} \tag{28}$$

where

$$\beta_{2\perp} \;=\; -\,\frac{1}{2}\,\tau^2 \;-\; \widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} \;+\; \langle\alpha_1^2\rangle \;-\; \left|\widehat{\mathsf{b}}\times\nabla\ln B\right|^2 \\ +\;\frac{1}{2}\,\widehat{\mathsf{b}}\cdot\nabla\times\left(\widehat{\mathsf{b}}\times\nabla\ln B\right), \qquad (29)$$

$$\beta_{2\|} \;=\; -\,2\,\langle\alpha_1^2\rangle \;-\; 3\,\boldsymbol{\kappa}\cdot\left(\nabla\ln B \;-\; \boldsymbol{\kappa}\right) \;+\; \nabla\cdot\boldsymbol{\kappa}, \quad (30)$$

with the definitions

$$\widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} \;=\; \frac{1}{2}\,\nabla\cdot\left[\boldsymbol{\kappa} \;-\; \widehat{\mathsf{b}}\,(\nabla\cdot\widehat{\mathsf{b}})\right], \qquad (31)$$

and

$$\langle\alpha_1^2\rangle \;=\; \frac{1}{2}\,\widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} \;+\; \frac{1}{8}\left[\tau^2 \;+\; \left(\nabla\cdot\widehat{\mathsf{b}}\right)^2\right]. \qquad (32)$$

The last term in Eq. (28) is also explicitly expressed as

$$\boldsymbol{\Pi}_1\cdot\mathbf{v}_{\rm gc} \;=\; \boldsymbol{\Pi}_{1\perp}\cdot\frac{\widehat{\mathsf{b}}}{m\Omega}\times\left(J\,\nabla\Omega \;+\; \frac{p_\|^2}{m}\,\boldsymbol{\kappa}\right). \qquad (33)$$

C. Previous second-order Hamiltonian representations

We now note that, in contrast to first-order guiding-center Hamiltonian constraint (23), the right side of Eq. (28) contains terms that are constant, quadratic, and quartic in $p_\|$. Hence, since Eq. (29) shows that $\beta_{2\perp} \neq 0$, we cannot choose $\Psi_2 = 0$ without making $\Pi_{2\|}$ singular in $p_\|$, i.e., a purely symplectic representation is no longer possible at second order.

In order to compare our results with the results presented in Refs. [1, 2], going back to Littlejohn's work [6], we choose $\Pi_{2\|} \equiv 0$ and $\boldsymbol{\Pi}_{1\perp} \equiv 0$ in Eq. (28). Hence, with these simplifying assumptions, our work agrees with the second-order guiding-center Hamiltonian of Burby, Squire, and Qin (BSQ) [2]:

$$\Psi_{2(TB)} \;=\; \Psi_{2(BSQ)} \;=\; \Psi_{2(PC)} \;+\; \frac{d_0\langle\sigma_3\rangle}{dt}, \qquad (34)$$

while it agrees with the second-order guiding-center Hamiltonian of Parra and Calvo (PC) [1] only up to the lowest-order guiding-center time derivative of the gyroangle-independent third-order gauge function

$$\langle\sigma_3\rangle \;=\; \frac{1}{2}\,J\,\varrho_\|\,(\nabla\cdot\widehat{\mathsf{b}}) \;\equiv\; \frac{d_0}{dt}\left(\frac{J}{2\Omega}\right) \qquad (35)$$

in the same manner discussed in Ref. [3], where $d_0\Omega^{-1}/dt = -\,\varrho_\|\,\widehat{\mathsf{b}}\cdot\nabla\ln B = \varrho_\|\,(\nabla\cdot\widehat{\mathsf{b}})$.

Lastly, in our previous work [11], where $\boldsymbol{\Pi}_{1\perp} \equiv 0$ was also assumed, we selected the following mixed representation: the second-order symplectic term

$$\Pi_{2\|}(p_\|, J, \mathbf{X}) \;=\; \frac{1}{2}\,p_\|\left(\varrho_\|^2|\boldsymbol{\kappa}|^2 \;-\; \frac{J\,\beta_{2\|}}{m\,\Omega}\right),$$

and the second-order Hamiltonian term $\Psi_2(J,\mathbf{X}) \equiv (J^2/2m)\,\beta_{2\perp}$, which follows from Eq. (28), was not included in Ref. [11].

D. Guiding-center transformation

The full Lie-transform perturbation analysis leading to the present higher-order guiding-center Hamiltonian theory will be presented in another publication. Here, we summarize the guiding-center phase-space transformation determined by the first-order generating vector-field components

$$G_1^{\mathbf{x}} \;=\; -\,\boldsymbol{\rho}_0, \qquad (36)$$

$$G_1^{p_\|} \;=\; -\,p_\|\,\boldsymbol{\rho}_0\cdot\boldsymbol{\kappa} \;+\; J\,(\tau \;+\; \alpha_1), \qquad (37)$$

$$G_1^J \;=\; \boldsymbol{\rho}_0\cdot\left(J\,\nabla\ln B + \frac{p_\|^2\,\boldsymbol{\kappa}}{m\Omega}\right) - J\,\varrho_\|\,(\tau+\alpha_1), \quad (38)$$

$$G_1^\theta \;=\; \varrho_\|\alpha_2 + \frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\left(\nabla\ln B + \frac{p_\|^2\boldsymbol{\kappa}}{2\,mJ\Omega} + \widehat{\mathsf{b}}\times\mathbf{R}\right) \quad (39)$$

where $\alpha_1 \equiv \partial\alpha_2/\partial\theta$, and the second-order generating vector-field components

$$G_2^{\mathbf{x}} \;=\; \left(2\,\varrho_\|\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\boldsymbol{\kappa} \;+\; \frac{J\,\alpha_2}{m\Omega}\right)\widehat{\mathsf{b}} \;-\; \boldsymbol{\Pi}_1\times\frac{\widehat{\mathsf{b}}}{m\Omega} \\ +\;\frac{1}{2}\left[\frac{p_\|^2}{m\Omega}\,(\boldsymbol{\rho}_0\cdot\boldsymbol{\kappa}) + J\,\varrho_\|\,(3\tau-\alpha_1)\right]\frac{\partial\boldsymbol{\rho}_0}{\partial J} \qquad (40) \\ +\;\frac{1}{2}\left[\varrho_\|\,\alpha_2 + \frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\left(\nabla\ln B + \frac{p_\|^2\,\boldsymbol{\kappa}}{2m\Omega\,J}\right)\right]\frac{\partial\boldsymbol{\rho}_0}{\partial\theta},$$

$$G_2^{p_\|} \;=\; p_\|\,\boldsymbol{\kappa}\cdot G_2^{\mathbf{x}} \;+\; \widehat{\mathsf{b}}\cdot\left[D_1^2(\mathbf{P}_3) + \nabla\sigma_3 - \boldsymbol{\Pi}_2\right], \qquad (41)$$

$$G_2^J \;=\; -\,\frac{1}{\Omega}\left(\Psi_2 \;-\; \frac{p_\|}{m}\,\Pi_{2\|}\right) - \varrho_\|\widehat{\mathsf{b}}\cdot\left[D_1^2(\mathbf{P}_3) + \nabla\sigma_3\right] \\ -G_2^{\mathbf{x}}\cdot\left(J\nabla\ln B + \frac{p_\|^2\,\boldsymbol{\kappa}}{m\,\Omega}\right), \qquad (42)$$

while

$$G_3^{\mathbf{x}} \;=\; G_{3\|}^{\mathbf{x}}\,\widehat{\mathsf{b}} \;+\; G_{2\|}^{\mathbf{x}}\left(\varrho_\|\,\nabla\times\widehat{\mathsf{b}}\right) \;-\; G_2^{\mathbf{x}}\left(\varrho_\|\,\tau\right) \\ -\;\frac{c\widehat{\mathsf{b}}}{eB}\times\left[D_1^2(\mathbf{P}_3) + \nabla\sigma_3 - \boldsymbol{\Pi}_2\right] \qquad (43)$$

is not needed in this Section. The remaining components $G_{3\|}^{\mathbf{x}}$ and G_2^θ, which are determined at fourth order, are not needed in what follows. In the expressions above, we used the definition

$$D_1(\cdots) \;\equiv\; \left(G_1^{p_\|}\frac{\partial}{\partial p_\|} + G_1^J\frac{\partial}{\partial J} + G_1^\theta\frac{\partial}{\partial\theta}\right)(\cdots) \\ +\;\boldsymbol{\rho}_0\times\nabla\times(\cdots),$$

and $\sigma_3 \equiv -\,\frac{1}{3}\,p_\|\;G_{2\|}^{\mathbf{x}}$ is the gyroangle-dependent gauge function that appears in the third-order Lie-transform perturbation analysis.

The guiding-center transformation presented above satisfies the first-order Jacobian constraint (20) and the second-order Jacobian constraint (21) consistent with the conditions $\Pi_{1\|} \equiv -\,\frac{1}{2}\,J\,\tau$ and $\partial\boldsymbol{\Pi}_1/\partial p_\| = 0$.

E. Push-forward Lagrangian Constraints

The second-order guiding-center Hamiltonian constraint (28) leads to a complex expression whose interpretation for Ψ_2 and $\Pi_{2\parallel}$ may be difficult to obtain. For this purpose, we wish to explore a new perturbation approach to guiding-center Hamiltonian theory.

We begin with the following remark for the phase-space Lagrangian formulation of single-particle dynamics in a potential $U(\mathbf{x})$, where the particle position $\mathbf{x}$ and its velocity $\mathbf{v}$ are viewed as independent phase-space coordinates. From the phase-space Lagrangian

$$L(\mathbf{x},\mathbf{v};\dot{\mathbf{x}},\dot{\mathbf{v}}) = \left(\frac{e}{c}\mathbf{A} + m\mathbf{v}\right)\boldsymbol{\cdot}\frac{d\mathbf{x}}{dt} - \left(\frac{m}{2}\,|\mathbf{v}|^2 + e\Phi\right),$$

we first obtain the Euler-Lagrange equation for $\mathbf{x}$: $m\,d\mathbf{v}/dt = e\,\mathbf{E} + \mathbf{v}\times e\,\mathbf{B}/c$. Since the phase-space Lagrangian is independent of $d\mathbf{v}/dt$, however, the Euler-Lagrange equation for $\mathbf{v}$ yields the Lagrangian constraint

$$\frac{\partial L}{\partial \mathbf{v}} \;=\; m\,\left(\frac{d\mathbf{x}}{dt} \;-\; \mathbf{v}\right) \;\equiv\; 0. \qquad (44)$$

Hence, the guiding-center transformation of the particle velocity $\mathbf{v}$ is constrained to be also expressed in terms of the guiding-center transformation of $d\mathbf{x}/dt$.

We would now like to obtain the guiding-center version of the Lagrangian constraint (44):

$$\mathsf{T}_{\rm gc}^{-1}\mathbf{p} \;=\; m\,\mathsf{T}^{-1}\left(\frac{d\mathbf{x}}{dt}\right) \;\equiv\; \mathbf{P}_{\rm gc}. \qquad (45)$$

First, using the functional definition for $d_{\rm gc}/dt$:

$$\frac{d_{\rm gc}}{dt} \;\equiv\; \mathsf{T}_{\rm gc}^{-1}\left(\frac{d}{dt}\,\mathsf{T}_{\rm gc}\right), \qquad (46)$$

we introduced in Eq. (45) the guiding-center particle-momentum

$$\mathbf{P}_{\rm gc} \;=\; m\,\frac{d_{\rm gc}}{dt}\left(\mathsf{T}_{\rm gc}^{-1}\mathbf{x}\right) = m\,\frac{d_{\rm gc}\mathbf{X}}{dt} + m\,\frac{d_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{dt}, \qquad (47)$$

which is expressed as the sum of the guiding-center velocity

$$\frac{d_{\rm gc}\mathbf{X}}{dt} \;=\; \frac{d_0\mathbf{X}}{dt} + \epsilon\,\frac{d_1\mathbf{X}}{dt} + \cdots \;=\; \frac{p_\parallel}{m}\,\widehat{\mathsf{b}} + \epsilon\,\mathbf{v}_{\rm gc} + \cdots$$

and the guiding-center displacement velocity

$$\frac{d_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{dt} = \epsilon^{-1}\,\frac{\partial\Psi}{\partial J}\,\frac{\partial\boldsymbol{\rho}_{\rm gc}}{\partial\theta} + \frac{d_{\rm gc}\mathbf{X}}{dt}\boldsymbol{\cdot}\nabla^*\boldsymbol{\rho}_{\rm gc} + \frac{d_{\rm gc}p_\parallel}{dt}\,\frac{\partial\boldsymbol{\rho}_{\rm gc}}{\partial p_\parallel},$$

where

$$\frac{d_{\rm gc}p_\parallel}{dt} \;=\; \frac{d_0p_\parallel}{dt} + \epsilon\,\frac{d_1p_\parallel}{dt} + \cdots \;=\; J\,\Omega\,\left(\nabla\boldsymbol{\cdot}\widehat{\mathsf{b}}\right) + \cdots.$$

Here, the guiding-center displacement is expanded as

$$\boldsymbol{\rho}_{\rm gc} \;\equiv\; \mathsf{T}_{\rm gc}^{-1}\mathbf{x} \,-\, \mathbf{X} \;=\; \epsilon\,\boldsymbol{\rho}_0 \,+\, \epsilon^2\,\boldsymbol{\rho}_1 \,+\, \epsilon^3\,\boldsymbol{\rho}_2 + \cdots, \qquad (48)$$

where the higher-order gyroradius corrections are

$$\boldsymbol{\rho}_1 \;=\; -\,G_2^{\mathbf{x}} \,-\, \frac{1}{2}\,\mathsf{G}_1\cdot\mathsf{d}\boldsymbol{\rho}_0, \qquad (49)$$

$$\boldsymbol{\rho}_2 \;=\; -\,G_3^{\mathbf{x}} - \mathsf{G}_2\cdot\mathsf{d}\boldsymbol{\rho}_0 + \frac{1}{6}\,\mathsf{G}_1\cdot\mathsf{d}(\mathsf{G}_1\cdot\mathsf{d}\boldsymbol{\rho}_0). \qquad (50)$$

We note that, in general, we find $\langle\boldsymbol{\rho}_n\rangle \neq 0$ and $\boldsymbol{\rho}_n\boldsymbol{\cdot}\widehat{\mathsf{b}} \neq 0$ for $n \geq 1$.

1. First-order Lagrangian constraint

The first-order Lagrangian constraints on the components $(G_1^{p_\parallel}, G_1^J, G_1^\theta)$ are expressed as

$$G_1^{p_\parallel}\,\widehat{\mathsf{b}} + G_1^J\,\frac{\partial\mathbf{p}_\perp}{\partial J} + G_1^\theta\,\frac{\partial\mathbf{p}_\perp}{\partial\theta} - \boldsymbol{\rho}_0\boldsymbol{\cdot}\nabla\mathbf{p} + \mathbf{P}_{\rm gc1} \;\equiv\; 0, \qquad (51)$$

where

$$\mathbf{P}_{\rm gc1} \equiv m\,\frac{d_1\mathbf{X}}{dt} \;+\; m\,\left(\frac{d_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{dt}\right)_1,$$

with

$$\left(\frac{d_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{dt}\right)_1 \;\equiv\; \Omega\,\frac{\partial\boldsymbol{\rho}_1}{\partial\theta} \;+\; \frac{d_0\boldsymbol{\rho}_0}{dt},$$

and

$$\frac{d_0\boldsymbol{\rho}_0}{dt} \;\equiv\; \frac{p_\parallel}{m}\widehat{\mathsf{b}}\boldsymbol{\cdot}\left[\nabla\boldsymbol{\rho}_0 \;+\; \left(\mathbf{R} + \frac{\partial\mathbf{\Pi}_1}{\partial J}\right)\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right].$$

Using the identity

$$\Psi_1 \;=\; \left\langle\mathbf{p}_\perp\boldsymbol{\cdot}\left(\frac{d_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{dt}\right)_1\right\rangle \;\equiv\; 0,$$

which follows from the first-order symplectic representation (24), Eq. (51) yields the same condition used in the first-order Hamiltonian constraint (23):

$$\langle G_1^J\rangle \;=\; \left\langle\boldsymbol{\rho}_0\boldsymbol{\cdot}\nabla\mathbf{p}\boldsymbol{\cdot}\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right\rangle \;=\; -\,J\,\varrho_\parallel\tau, \qquad (52)$$

which is calculated at order ϵ^3 in the Lie-transform perturbation analysis.

2. Second-order Lagrangian constraint

The second-order components $(G_2^{p_\parallel}, G_2^J, G_2^\theta)$ are also constrained by the second-order Lagrangian constraint

$$G_2^{p_\parallel}\,\widehat{\mathsf{b}} \,+\, G_2^J\,\frac{\partial\mathbf{p}_\perp}{\partial J} \,+\, G_2^\theta\,\frac{\partial\mathbf{p}_\perp}{\partial\theta} \,+\, G_2^{\mathbf{x}}\boldsymbol{\cdot}\nabla\mathbf{p}$$
$$-\,\frac{1}{2}\,\mathsf{G}_1\cdot\mathsf{d}\left(\mathsf{G}_1\cdot\mathsf{d}\mathbf{p}\right) \,+\, \mathbf{P}_{\rm gc2} \;\equiv\; 0, \qquad (53)$$

where

$$\mathbf{P}_{\rm gc2} \;\equiv\; m\,\frac{d_2\mathbf{X}}{dt} + m\,\left(\frac{d_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{dt}\right)_2$$

with

$$\left(\frac{d_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{dt}\right)_2 \equiv \Omega\,\frac{\partial\boldsymbol{\rho}_2}{\partial\theta} + \frac{\partial\Psi_2}{\partial J}\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} + \frac{d_1\mathbf{X}}{dt}\boldsymbol{\cdot}\nabla_0^*\boldsymbol{\rho}_0 + \frac{d_0\boldsymbol{\rho}_1}{dt},$$

and

$$\frac{d_0\boldsymbol{\rho}_1}{dt} \;=\; \frac{p_\|}{m}\widehat{\sf b}\boldsymbol{\cdot}\left[\nabla\boldsymbol{\rho}_1 \;+\; \left(\mathbf{R} + \frac{\partial\boldsymbol{\Pi}_1}{\partial J}\right)\frac{\partial\boldsymbol{\rho}_1}{\partial\theta}\right] + \left[J\,\Omega\,\left(\nabla\boldsymbol{\cdot}\widehat{\sf b}\right)\right]\,\frac{\partial\boldsymbol{\rho}_1}{\partial p_\|}.$$

In particular, the Lagrangian constraint on $\langle G_2^J\rangle$ yields

$$\langle G_2^J\rangle \;=\; -\left\langle G_2^{\bf x}\boldsymbol{\cdot}\nabla\mathbf{p}\boldsymbol{\cdot}\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right\rangle - m\left\langle\left(\frac{d_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{dt}\right)_2\boldsymbol{\cdot}\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right\rangle + \frac{1}{2}\left\langle\left[{\sf G}_1\cdot{\sf d}\;({\sf G}_1\cdot{\sf d}\mathbf{p})\right]\boldsymbol{\cdot}\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right\rangle, \tag{54}$$

which yields the same result as Eq. (27) obtained at order ϵ^4 in the Lie-transform perturbation analysis.

3. Lagrangian constraint on the guiding-center Hamiltonian

The generating-field components (36)-(42) were shown to satisfy the guiding-center Lagrangian constraints (51)-(53). This means that the guiding-center Hamiltonian

$$H_{\rm gc} \;\equiv\; \frac{m}{2}\left\langle\left|\frac{d_{\rm gc}\mathbf{X}}{dt} \;+\; \frac{d_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{dt}\right|^2\right\rangle, \tag{55}$$

can also be expressed in terms of guiding-center velocity $d_{\rm gc}\mathbf{X}/dt$ and the guiding-center displacement velocity $d_{\rm gc}\boldsymbol{\rho}_{\rm gc}/dt$. In the second-order Hamiltonian representation ($\Pi_{2\|}\equiv 0$), the Lagrangian constraint of the guiding-center Hamiltonian (55) implies that

$$\Psi_2 \equiv \epsilon^{-2}\left[\frac{p_\|^2}{2m} + J\,\Omega - \frac{m}{2}\left\langle\left|\frac{d_{\rm gc}\mathbf{X}}{dt} + \frac{d_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{dt}\right|^2\right\rangle\right], \tag{56}$$

which is identical to Eq. (28) (with $\Pi_{2\|}\equiv 0$).

IV. GUIDING-CENTER POLARIZATION AND TOROIDAL CANONICAL MOMENTUM

There is now well-established connection between polarization and the conservation of toroidal canonical momentum in an axisymmetric magnetic field. We now show how $\boldsymbol{\Pi}_{1\perp}$, which was originally chosen by Littlejohn [6] to be zero, can be determined by requiring that the guiding-center transformation (17) yields the guiding-center polarization obtained by Pfirsch [8] and Kaufman [9]. We will also show that the *polarization* term $\boldsymbol{\Pi}_{1\perp}$ leads to a more transparent guiding-center representation of the toroidal canonical angular momentum in axisymmetric magnetic geometry.

A. Guiding-center polarization

The guiding-center transformation (17) can be used to calculate polarization and magnetization effects associated with the guiding-center displacement $\boldsymbol{\rho}_{\rm gc}$, defined by Eq. (48).

Since the dipole contribution to the guiding-center polarization [10] involves the gyroangle-averaged displacement $\langle\boldsymbol{\rho}_{\rm gc}\rangle = \epsilon^2\,\langle\boldsymbol{\rho}_1\rangle + \cdots$ (since $\langle\boldsymbol{\rho}_0\rangle\equiv 0$), we begin with the gyroangle-averaged first-order displacement calculated from Eq. (49):

$$\begin{aligned}\langle\boldsymbol{\rho}_1\rangle \;&=\; -\,\frac{J}{m\Omega}\left[\frac{1}{2}\,(\nabla\boldsymbol{\cdot}\widehat{\sf b})\,\widehat{\sf b} \;+\; \frac{3}{2}\,\nabla_\perp\ln B\right] - \varrho_\|^2\,\boldsymbol{\kappa} \;+\; \boldsymbol{\Pi}_1\times\frac{\widehat{\sf b}}{m\Omega}\\ &\equiv\; -\,\frac{1}{m\Omega}\left(J\,\nabla_\perp\ln B + \frac{p_\|^2\,\boldsymbol{\kappa}}{m\,\Omega}\right) + \nabla\boldsymbol{\cdot}\left(\left\langle\frac{\boldsymbol{\rho}_0\boldsymbol{\rho}_0}{2}\right\rangle\right) + \left(\frac{J}{2}\,\widehat{\sf b}\times\boldsymbol{\kappa} \;+\; \boldsymbol{\Pi}_1\right)\times\frac{\widehat{\sf b}}{m\Omega},\end{aligned} \tag{57}$$

where we used Eqs. (36)-(40), with

$$\begin{aligned}\nabla\boldsymbol{\cdot}\left(\left\langle\frac{\boldsymbol{\rho}_0\boldsymbol{\rho}_0}{2}\right\rangle\right) \;&=\; \nabla\boldsymbol{\cdot}\left[\frac{J}{2\,m\Omega}\,\left(\mathbf{I} - \widehat{\sf b}\widehat{\sf b}\right)\right]\\ &=\; -\,\frac{J}{2\,m\Omega}\left[\boldsymbol{\kappa} + \nabla_\perp\ln B \;+\; (\nabla\boldsymbol{\cdot}\widehat{\sf b})\,\widehat{\sf b}\right].\end{aligned}$$

Next, the guiding-center polarization density is defined as the first-order expression [10]

$$\begin{aligned}\boldsymbol{\pi}_{\rm gc}^{(1)} \;&\equiv\; e\,\langle\boldsymbol{\rho}_1\rangle \;-\; e\,\nabla\boldsymbol{\cdot}\left(\left\langle\frac{\boldsymbol{\rho}_0\boldsymbol{\rho}_0}{2}\right\rangle\right)\\ &=\; -\,\frac{e}{m\Omega}\left(J\,\nabla_\perp\ln B \;+\; \frac{p_\|^2\,\boldsymbol{\kappa}}{m\,\Omega}\right) + \left(\frac{J}{2}\,\widehat{\sf b}\times\boldsymbol{\kappa} \;+\; \boldsymbol{\Pi}_1\right)\times\frac{c\widehat{\sf b}}{B},\end{aligned} \tag{58}$$

which yields the Pfirsch-Kaufman formula [8, 9]

$$\boldsymbol{\pi}_{\rm gc}^{(1)} \;\equiv\; e\,\widehat{\sf b}\times\frac{1}{\Omega}\frac{d_1\mathbf{X}}{dt} \;=\; e\,\widehat{\sf b}\times\frac{\mathbf{v}_{\rm gc}}{\Omega}, \tag{59}$$

only if we use the definition

$$\boldsymbol{\Pi}_{1\perp} \;\equiv\; -\,\frac{J}{2}\,\widehat{\sf b}\times\boldsymbol{\kappa}. \tag{60}$$

Hence, by combining with the condition (24), $\Pi_{1\|}\equiv\widehat{\sf b}\boldsymbol{\cdot}\boldsymbol{\Pi}_1 = -\,\frac{1}{2}\,J\,\tau$, we find

$$\boldsymbol{\Pi}_1 \;=\; -\,\frac{J}{2}\left(\tau\,\widehat{\sf b} \;+\; \widehat{\sf b}\times\boldsymbol{\kappa}\right) \;=\; -\,\frac{J}{2}\,\nabla\times\widehat{\sf b}, \tag{61}$$

which satisfies the Jacobian constraint (22). We note that the Pfirsch-Kaufman formula (59) yields a guiding-center moving-electric-dipole correction $\boldsymbol{\mu}_{\rm gc}^{(E)}\equiv p_\|\mathbf{v}_{\rm gc}/B$

to the intrinsic guiding-center magnetic-dipole moment $\boldsymbol{\mu}_{\rm gc}^{(B)} \equiv -\,\mu\,\widehat{\sf b}$.

Lastly, the guiding-center phase-space Lagrangian is expressed as

$$\Gamma_{\rm gc} \;=\; \left(\frac{e}{\epsilon\, c}\,\mathbf{A} \;+\; p_{\|}\,\widehat{\sf b} \;-\; \frac{\epsilon}{2}\,J\,\nabla\times\widehat{\sf b}\right)\cdot{\sf d}\mathbf{X} \;+\; \epsilon\,J\;\left({\sf d}\theta \;-\; \mathbf{R}\cdot{\sf d}\mathbf{X}\right), \qquad (62)$$

when terms up to first order in magnetic-field nonuniformity are retained. In Eq. (62), we have retained the guiding-center polarization contribution to $\mathbf{\Pi}_1 \equiv -\frac{1}{2}\,J\,\nabla\times\widehat{\sf b}$. We now show that this polarization correction yields a more transparent expression for the guiding-center toroidal canonical momentum up to second order in ϵ (i.e., first order in magnetic-field nonuniformity).

B. Guiding-center toroidal canonical angular momentum

We now construct the guiding-center representation for the toroidal canonical angular momentum in axisymmetric magnetic geometry, for which it is an exact constant of motion. Here, we represent an axisymmetric magnetic field

$$\mathbf{B} \;=\; B_{\varphi}(\psi)\,\nabla\varphi \;+\; \nabla\varphi\times\nabla\psi, \qquad (63)$$

where φ denotes the toroidal angle and ψ denotes the magnetic flux on which magnetic-field lines lie (i.e., $\mathbf{B}\cdot\nabla\psi \equiv 0$). Note that we have added a toroidal magnetic field $B_{\varphi}\,\nabla\varphi$ in Eq. (63), with a covariant component B_{φ} that is constant on a given magnetic-flux surface.

We first calculate the guiding-center toroidal canonical momentum from the guiding-center phase-space Lagrangian (62):

$$\begin{aligned} P_{{\rm gc}\varphi} \;&\equiv\; \left[\frac{e}{\epsilon\, c}\,\mathbf{A} + p_{\|}\,\widehat{\sf b} - \epsilon\,J\,\left(\mathbf{R} + \frac{1}{2}\,\nabla\times\widehat{\sf b}\right)\right]\cdot\frac{\partial\mathbf{X}}{\partial\varphi} \\ &=\; -\frac{e}{\epsilon\, c}\,\psi + p_{\|}\,b_{\varphi} - \epsilon\,J\left[b_{\sf z} + \widehat{\sf b}\cdot\nabla\times\left(\frac{1}{2}\,\mathcal{R}^2\,\nabla\varphi\right)\right] \\ &\quad -\,\epsilon\,J\nabla\cdot\left(\widehat{\sf b}\times\frac{1}{2}\,\mathcal{R}^2\,\nabla\varphi\right) \end{aligned} \qquad (64)$$

where we used $\mathbf{R}\cdot\partial\mathbf{X}/\partial\varphi \equiv b_{\sf z}$ [6] (i.e., the component of $\widehat{\sf b}$ along the symmetry axis $\widehat{\sf z}$ for toroidal rotations), we wrote $\partial\mathbf{X}/\partial\varphi \equiv \mathcal{R}^2\,\nabla\varphi$ in terms of the major radius $\mathcal{R} \equiv |\nabla\varphi|^{-1}$, and we used the identity $\mathbf{F}\cdot\nabla\times\mathbf{G} \equiv \nabla\cdot(\mathbf{G}\times\mathbf{F}) + \mathbf{G}\cdot\nabla\times\mathbf{F}$, for arbitrary vector fields $\mathbf{F}$ and $\mathbf{G}$. Next, we use

$$\widehat{\sf b}\cdot\nabla\times\left(\frac{1}{2}\,\mathcal{R}^2\,\nabla\varphi\right) \;=\; \widehat{\sf b}\cdot\left(\widehat{\mathcal{R}}\times\widehat{\varphi}\right) \;=\; b_{\sf z},$$

and

$$\widehat{\sf b}\times\frac{1}{2}\,\mathcal{R}^2\,\nabla\varphi \;=\; \frac{1}{2B}\,\nabla\psi,$$

so that Eq. (64) becomes

$$\begin{aligned} P_{{\rm gc}\varphi} \;&=\; -\,\frac{e}{\epsilon\, c}\,\left[\psi \;+\; \epsilon^2\,\nabla\cdot\left(\frac{J}{2\,m\Omega}\,\nabla\psi\right)\right] \\ &\quad +\, p_{\|}\,b_{\varphi} \;-\; 2\,\epsilon\,J\,b_{\sf z}. \end{aligned} \qquad (65)$$

Here, the second term on the first line in Eq. (65) is the second-order finite-Larmor-radius (FLR) correction to the first term.

We now show that Eq. (65) is the exact guiding-center representation of the toroidal canonical angular momentum:

$$P_{{\rm gc}\varphi} \equiv {\sf T}_{\rm gc}^{-1}P_{\varphi} = -\,\frac{e}{c\epsilon}\,{\sf T}_{\rm gc}^{-1}\psi + {\sf T}_{\rm gc}^{-1}\left(m\,\mathbf{v}\cdot\frac{\partial\mathbf{x}}{\partial\varphi}\right), \quad (66)$$

which guarantees the conservation of guiding-center toroidal canonical angular momentum

$$\frac{d_{\rm gc}P_{{\rm gc}\varphi}}{dt} \;=\; \frac{d_{\rm gc}}{dt}\left({\sf T}_{\rm gc}^{-1}\,P_{\varphi}\right) \;=\; {\sf T}_{\rm gc}^{-1}\left(\frac{dP_{\varphi}}{dt}\right) \;\equiv\; 0. \quad (67)$$

First, we note that, while the term ${\sf T}_{\rm gc}^{-1}P_{\varphi}$ in Eq. (66) contains contributions that are gyroangle-independent and contributions that are explicitly gyroangle-dependent, the term $P_{{\rm gc}\varphi}$ is explicitly gyroangle-independent. Hence, the gyroangle-dependent contributions must vanish at all orders in ϵ, and thus $P_{{\rm gc}\varphi} \equiv \langle{\sf T}_{\rm gc}^{-1}P_{\varphi}\rangle$; this identity, which is equivalent to a toroidal-canonical-momentum constraint on the guiding-center transformation, will be proved elsewhere.

Secondly, we therefore introduce the guiding-center magnetic flux $\psi_{\rm gc} \equiv \langle{\sf T}_{\rm gc}^{-1}\psi\rangle$:

$$\begin{aligned} \psi_{\rm gc} \;&=\; \psi \;+\; \epsilon^2\left(\langle\boldsymbol{\rho}_1\rangle\cdot\nabla\psi \;+\; \frac{1}{2}\,\langle\boldsymbol{\rho}_0\boldsymbol{\rho}_0\rangle : \nabla\nabla\psi\right) + \cdots \\ &=\; \psi + \epsilon^2\,\nabla\cdot\left(\frac{J}{2\,m\Omega}\,\nabla\psi\right) + \epsilon^2\,\widehat{\sf b}\times\frac{\mathbf{v}_{\rm gc}}{\Omega}\cdot\nabla\psi, \end{aligned} \quad (68)$$

where we used Eqs. (57)-(59). In Eq. (68), the second term is an FLR correction to the first term, while the last term is easily recognized as a correction due to the guiding-center polarization (59).

Thirdly, using the identity $\nabla\psi \equiv \mathbf{B}\times\partial\mathbf{X}/\partial\varphi$, with $\widehat{\sf b}\cdot\mathbf{v}_{\rm gc} \equiv 0$, we obtain

$$\widehat{\sf b}\times\frac{\mathbf{v}_{\rm gc}}{\Omega}\cdot\nabla\psi \;=\; \frac{B}{\Omega}\,\left(\mathbf{v}_{\rm gc}\cdot\frac{\partial\mathbf{X}}{\partial\varphi}\right) \;\equiv\; \frac{B}{\Omega}\,v_{{\rm gc}\varphi}.$$

Hence, the final expression for the guiding-center toroidal canonical momentum defined by Eq. (65) is

$$P_{{\rm gc}\varphi} \;=\; -\,\frac{e}{\epsilon\, c}\,\psi_{\rm gc} + m\left(\frac{d_0\mathbf{X}}{dt} + \epsilon\,\frac{d_1\mathbf{X}}{dt}\right)\cdot\frac{\partial\mathbf{X}}{\partial\varphi} - 2\,\epsilon\,J\,b_{\sf z}, \qquad (69)$$

where $d_0\mathbf{X}/dt \equiv (p_{\|}/m)\,\widehat{\sf b}$ and $d_1\mathbf{X}/dt \equiv \mathbf{v}_{\rm gc}$, while

$$m\,\left(\frac{d_0\mathbf{X}}{dt} \;+\; \epsilon\,\frac{d_1\mathbf{X}}{dt}\right)\cdot\frac{\partial\mathbf{X}}{\partial\varphi} \;\equiv\; m\,\mathcal{R}^2\,\frac{d_{\rm gc}\varphi}{dt}$$

denotes the guiding-center toroidal momentum with first-order corrections due to the guiding-center magnetic-drift velocity.

The last term in Eq. (69) might be puzzling until we consider the guiding-center transformation of the particle toroidal canonical momentum $P_{{\rm gc}\varphi} \equiv \langle \mathsf{T}_{\rm gc}^{-1}\, p_\varphi\rangle$:

$$\begin{aligned} P_{{\rm gc}\varphi} &= -\,\frac{e}{\epsilon\, c}\,\langle \mathsf{T}_{\rm gc}^{-1}\psi\rangle \;+\; m\,\left\langle\left(\mathsf{T}_{\rm gc}^{-1}\frac{d\mathbf{x}}{dt}\right)\cdot\left(\mathsf{T}_{\rm gc}^{-1}\frac{\partial\mathbf{x}}{\partial\varphi}\right)\right\rangle \\ &= -\,\frac{e}{\epsilon\, c}\,\psi_{\rm gc} \;+\; m\left(\frac{d_0\mathbf{X}}{dt} \;+\; \epsilon\,\frac{d_1\mathbf{X}}{dt}\right)\cdot\frac{\partial\mathbf{X}}{\partial\varphi} \\ &\quad +\,\epsilon\, m\Omega\left\langle\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\frac{\partial\boldsymbol{\rho}_0}{\partial\varphi}\right\rangle + \cdots . \end{aligned} \tag{70}$$

Since $\partial\boldsymbol{\rho}_0/\partial\varphi \equiv \widehat{\mathsf{z}}\times\boldsymbol{\rho}_0$ in axisymmetric magnetic geometry, the last term in Eq. (70) becomes

$$\epsilon\, m\Omega\left\langle\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\frac{\partial\boldsymbol{\rho}_0}{\partial\varphi}\right\rangle \;=\; -\,2\,\epsilon\, J\, b_{\mathsf{z}},$$

and we recover the guiding-center toroidal canonical momentum (69) from the guiding-center transformation of the particle toroidal canonical momentum (70).

C. Comparison with Littlejohn's results

By comparison, the guiding-center toroidal canonical momentum obtained by Littlejohn [6] and all subsequent guiding-center theories, is calculated with the choice $\mathbf{\Pi}_{1\perp} \equiv 0$:

$$(P_{{\rm gc}\varphi})_{\rm RGL} \;=\; -\,\frac{e}{\epsilon\, c}\,\psi \;+\; p_\|\, b_\varphi \;+\; \epsilon\left(\Pi_{1\|}\, b_\varphi \;-\; J\, b_{\mathsf{z}}\right), \tag{71}$$

where the FLR correction to ψ and the missing additional b_{z}-term are hidden in $\Pi_{1\|}\, b_\varphi \equiv -\,\frac{1}{2}\,J\,\tau\, b_\varphi$:

$$\begin{aligned} -\,\frac{1}{2}\,J\,\tau\, b_\varphi &= -\,\frac{1}{2}\,J\left(\nabla\times\widehat{\mathsf{b}}\cdot\frac{\partial\mathbf{X}}{\partial\varphi} \;+\; \widehat{\mathsf{b}}\times\frac{\partial\mathbf{X}}{\partial\varphi}\cdot\boldsymbol{\kappa}\right) \\ &= -\,\nabla\cdot\left(\frac{J}{2B}\,\nabla\psi\right) \;-\; J\, b_{\mathsf{z}} \;-\; \frac{J}{2B}\,\boldsymbol{\kappa}\cdot\nabla\psi. \end{aligned}$$

Hence, the Littlejohn guiding-center toroidal canonical momentum (71) becomes

$$\begin{aligned} (P_{{\rm gc}\varphi})_{\rm RGL} &= -\,\frac{e}{\epsilon\, c}\left[\psi \;+\; \epsilon^2\,\nabla\cdot\left(\frac{J}{2\,m\Omega}\,\nabla\psi\right)\right] \\ &\quad + p_\|\, b_\varphi - \epsilon\left(2\,J\, b_{\mathsf{z}} + \frac{J\boldsymbol{\kappa}}{2B}\cdot\nabla\psi\right). \end{aligned} \tag{72}$$

We note that Belova *et al.* [13] have shown that the second-order (ϵ^2) corrections to the guiding-center toroidal canonical momentum (71) were shown to be crucial in satisfying the conservation of toroidal canonical momentum in realistic axisymmetric tokamak plasmas.

The Littlejohn guiding-center toroidal canonical momentum (72), of course, has the same form as Eq. (69) since its associated guiding-center magnetic flux is

$$\begin{aligned} (\psi_{\rm gc})_{\rm RGL} &= \psi \;+\; \epsilon^2\,\nabla\cdot\left(\frac{J}{2\,m\Omega}\,\nabla\psi\right) \\ &\quad +\,\epsilon^2\left(\widehat{\mathsf{b}}\times\frac{\mathbf{v}_{\rm gc}}{\Omega} \;+\; \frac{J\boldsymbol{\kappa}}{2m\Omega}\right)\cdot\nabla\psi \\ &\equiv \psi_{\rm gc} \;+\; \epsilon^2\,\frac{J\,\boldsymbol{\kappa}}{2\,m\Omega}\cdot\nabla\psi, \end{aligned} \tag{73}$$

where the extra term associated with the normal magnetic curvature $\boldsymbol{\kappa}\cdot\nabla\psi/|\nabla\psi|$ was eliminated by our choice (60) for $\mathbf{\Pi}_{1\perp}$.

We, therefore, conclude that the exact guiding-center representation (65) [or (69)] of the toroidal canonical angular momentum in axisymmetric magnetic geometry requires that the calculation of the guiding-center transformation must retain the perpendicular component $\mathbf{\Pi}_{1\perp}$, as defined by Eq. (61) through the calculation of the guiding-center polarization, and properly included in the guiding-center symplectic structure (62).

V. SUMMARY

In conclusion, a systematic derivation of the Hamiltonian guiding-center dynamics has been derived by Lie-transform perturbation analysis. The guiding-center Poisson bracket derived from the guiding-center phase-space Lagrangian (62) and the guiding-center Hamiltonian (55). These guiding-center Hamilton equations have passed several consistency tests along the way.

First, we verified that our guiding-center transformation satisfies the guiding-center Jacobian constraints at first and second orders. Next, we verified that our guiding-center transformation also satisfy the guiding-center Lagrangian constraints at first and second orders. In fact, the use of the Lagrangian constraints on the guiding-center transformation yields a natural expression (55) for the guiding-center Hamiltonian in terms of the guiding-center velocity $d_{\rm gc}\mathbf{X}/dt$ and the guiding-center displacement velocity $d_{\rm gc}\boldsymbol{\rho}_{\rm gc}/dt$. When the polarization term $\mathbf{\Pi}_{1\perp}$ is ignored in the guiding-center Hamiltonian, our second-order guiding-center Hamiltonian is identical to the Hamiltonian derived by Burby, Squire, and Qin [2].

We also showed that the perpendicular component of $\mathbf{\Pi}_1$, which could not be determined at the perturbation orders considered in this work, could nevertheless not be chosen to be zero, in contrast to the simplifying choice made by Littlejohn [6]. The choice (61) defined in the present work not only yields the standard Pfirsch-Kaufman guiding-center polarization (59), but also yields a simpler and more transparent guiding-center representation of the particle toroidal canonical momentum (69).

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