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Equivalent Higher-order 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 an exact (and more transparent) 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.

1. 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.

Recently, Parra and Calvo (Parra & Calvo 2011) and Burby, Squire, and Qin (Burby *et al.* 2013) derived guiding-center theories with second-order corrections in the guiding-center Hamiltonian using different methods. Parra and Calvo (Parra & Calvo 2011) 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 $\rho_{\rm g}$ to the magnetic nonuniformity length scale $L_{\rm B}$. Burby, Squire, and Qin (Burby *et al.* 2013) , on the other hand, derived the second-order guiding-center Hamiltonian through a computer-based algorithm that bypassed the issue of gyrogauge invariance.

These theories were compared by Parra, Calvo, Burby, Squire, and Qin (Parra *et al.* 2014) 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 ((Littlejohn 1979), (Littlejohn 1981), & (Littlejohn 1983)),

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which made certain simplifying assumptions on the symplectic part of the guiding-center phase-space Lagrangian.

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. In the process, we show that a consistent treatment of guiding-center polarization and the accurate guiding-center representation of the toroidal canonical angular momentum, which is an exact constant of motion in axisymmetric magnetic geometry, requires that a new first-order term be kept in the symplectic part of the guiding-center phase-space Lagrangian. We also introduced two new constraints on the guiding-center transformation that guarantee the consistency of the guiding-center Hamilton equations.

The material contained in this manuscript is presented in tutorial form, with detailed calculations appearing for the first time. The remainder of the paper is organized as follows. In Sec. 2, we present a summary of the general formulation of guiding-center Hamiltonian theory, in which corrections associated with magnetic-field nonuniformity appear at all orders in the guiding-center Hamiltonian and/or the guiding-center Poisson bracket. In Sec. 3, the formulation of Lie-transform perturbation theory for the Lagrange one-form is presented up to fourth order in the ordering parameter ϵ, which are explicitly solved in Secs. 4-7. The ordering parameter ϵ is used in the renormalization of the electric charge $e \rightarrow e/\epsilon$ that appears in the *macroscopic* view of guiding-center dynamics, in which the magnetic-nonuniformity length scale is finite while the gyroradius is small. In Secs. 8-9, we present the Jacobian and Lagrangian constraints that establish the consistency of the guiding-center phase-space transformation. In Sec. 10, we derive the guiding-center polarization directly from the guiding-center transformation, which further constrains the transformation, and discuss the conservation of the guiding-center toroidal canonical momentum. In Sec. 11, we summarize our work. Lastly, the Appendices A-G provide a wealth of results that support the material presented in the text.

2. Guiding-center Hamiltonian Theory

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 $p_{\|}$, and the guiding-center gyroaction $J \equiv \mu\, B/\Omega$ (defined in terms of the guiding-center magnetic moment μ and the gyrofrequency $\Omega = eB/mc$ for a particle of mass m and charge e); it is, however, independent of the gyroangle θ at all orders. Since the guiding-center phase-space coordinates are non-canonical coordinates, a noncanonical guiding-center Poisson bracket is also needed. In what follows, we use the macroscopic view whereby an ordering parameter ϵ is introduced by renormalizing the electric charge $e \rightarrow e/\epsilon$ (e.g., $\Omega \rightarrow \epsilon^{-1}\Omega$ and $J \rightarrow \epsilon\, J$).

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

$$H_{\rm gc} \;\equiv\; \frac{p_{\|}^{2}}{2m} \;+\; \Psi, \tag{2.1}$$

where the effective guiding-center potential energy

$$\Psi \;\equiv\; J\,\Omega \;+\; \epsilon\,\Psi_{1} \;+\; \epsilon^{2}\,\Psi_{2} \;+\; \cdots \tag{2.2}$$

is defined in terms of higher-order corrections Ψ_n $(n \geq 1)$ that vanish in a uniform magnetic field. The guiding-center symplectic structure, on the other hand, is expressed in terms of the guiding-center Poincaré-Cartan one-form

$$\Gamma_{\rm gc} \equiv \left(\frac{e}{\epsilon c}\,\mathbf{A} \;+\; \mathbf{\Pi}\right)\boldsymbol{\cdot}\mathsf{d}\mathbf{X} \;+\; \epsilon\,J\,(\mathsf{d}\theta \;-\; \mathbf{R}\boldsymbol{\cdot}\mathsf{d}\mathbf{X})\,, \tag{2.3}$$

where the symplectic guiding-center momentum

$$\mathbf{\Pi} \;\equiv\; \sum_{n=0}^{\infty}\epsilon^{n}\,\mathbf{\Pi}_{n} \;=\; p_{\|}\,\widehat{\mathsf{b}} \;+\; \epsilon\,\mathbf{\Pi}_{1} \;+\; \epsilon^{2}\,\mathbf{\Pi}_{2} + \cdots \tag{2.4}$$

is expressed in terms of the gyroangle-independent vector terms $\mathbf{\Pi}_n$ ($n \geq 1$), which contain corrections due to magnetic-field nonuniformity, and the presence of the gyrogauge vector $\mathbf{R}$ guarantees that the the guiding-center one-form (2.3) is gyrogauge-invariant. We note that the guiding-center phase-space Lagrangian

$$\begin{aligned}\Gamma_{\rm gc} \;-\; H_{\rm gc}\,\mathsf{d}t \equiv & \left[\left(\frac{e}{\epsilon c}\,\mathbf{A} + p_{\|}\,\widehat{\mathsf{b}}\right)\boldsymbol{\cdot}\mathsf{d}\mathbf{X} \;+\; \epsilon\,J\,\left(\mathsf{d}\theta \;-\; \mathbf{R}\boldsymbol{\cdot}\mathsf{d}\mathbf{X}\right)\right] \;-\; \left(\frac{p_{\|}^{2}}{2m} \;+\; J\,\Omega\right)\mathsf{d}t \\ & +\; \sum_{n=1}^{\infty}\epsilon^{n}\left(\mathbf{\Pi}_{n}\boldsymbol{\cdot}\mathsf{d}\mathbf{X} \;-\; \Psi_{n}\;\mathsf{d}t\right)\end{aligned} \tag{2.5}$$

can either be derived simultaneously or separately.

The guiding-center Poisson bracket obtained from the guiding-center Euler-Poincaré one-form (2.3) by following the following inversion procedure. First, we construct the guiding-center Lagrange two-form

$$\boldsymbol{\omega}_{\rm gc} \equiv \mathsf{d}\Gamma_{\rm gc} = \frac{eB^{*k}}{2\,\epsilon c}\,\varepsilon_{ijk}\;\mathsf{d}X^{i}\wedge\mathsf{d}X^{j} + \mathsf{d}p_{\|}\wedge\widehat{\mathsf{b}}^{*}\boldsymbol{\cdot}\mathsf{d}\mathbf{X} + \epsilon\mathbf{R}^{*}\boldsymbol{\cdot}\mathsf{d}\mathbf{X}\wedge\mathsf{d}J + \epsilon\mathsf{d}J\wedge\mathsf{d}\theta,$$

where ε_{ijk} denotes the Levi-Civita tensor. We note that the Lagrange component-matrix is invertible since the guiding-center Jacobian

$$\mathcal{J}_{\rm gc} \;\equiv\; \sqrt{\det(\boldsymbol{\omega}_{\rm gc})} \;=\; \epsilon\;\widehat{\mathsf{b}}^{*}\boldsymbol{\cdot}\left(\frac{e}{\epsilon\,c}\;\mathbf{B}^{*}\right) \;\equiv\; \frac{e}{c}\;B_{\|}^{**} \;\neq\; 0, \tag{2.6}$$

with the following definitions

$$\mathbf{B}^{*} \equiv \nabla\times\left[\mathbf{A} \;+\; \frac{c}{e}\;\left(\epsilon\,\mathbf{\Pi} \;-\; \epsilon^{2}\;J\;\mathbf{R}\right)\right], \tag{2.7}$$

$$\widehat{\mathsf{b}}^{*} \equiv \frac{\partial\mathbf{\Pi}}{\partial p_{\|}} \;=\; \widehat{\mathsf{b}} \;+\; \epsilon\;\frac{\partial\mathbf{\Pi}_{1}}{\partial p_{\|}} \;+\; \epsilon^{2}\;\frac{\partial\mathbf{\Pi}_{2}}{\partial p_{\|}} \;+\; \cdots\,, \tag{2.8}$$

$$\mathbf{R}^{*} \equiv \mathbf{R} \;-\; \epsilon^{-1}\;\frac{\partial\mathbf{\Pi}}{\partial J} \;=\; \mathbf{R} \;-\; \frac{\partial\mathbf{\Pi}_{1}}{\partial J} \;-\; \epsilon\;\frac{\partial\mathbf{\Pi}_{2}}{\partial J} \;+\; \cdots\,, \tag{2.9}$$

$$B_{\|}^{**} \equiv \widehat{\mathsf{b}}^{*}\boldsymbol{\cdot}\mathbf{B}^{*} = \left(\widehat{\mathsf{b}} + \epsilon\frac{\partial\mathbf{\Pi}_{1}}{\partial p_{\|}} + \cdots\right)\boldsymbol{\cdot}\mathbf{B}^{*}. \tag{2.10}$$

Here the fields $\mathbf{B}^{*}$ and $\widehat{\mathsf{b}}^{*}$ satisfy the identities

$$\left.\begin{aligned}\nabla\boldsymbol{\cdot}\mathbf{B}^{*} \;&\equiv\; 0 \\ \partial\mathbf{B}^{*}/\partial p_{\|} \;&\equiv\; \epsilon\,(c/e)\,\nabla\times\widehat{\mathsf{b}}^{*}\end{aligned}\right\}, \tag{2.11}$$

which will play an important role in the properties of the guiding-center Poisson bracket.

Next, we invert the guiding-center Lagrange matrix 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 $\{F,\,G\}_{\rm gc} \equiv (\partial F/\partial Z^{\alpha})\,J_{\rm gc}^{\alpha\beta}\,(\partial G/\partial Z^{\beta})$:

$$\Big\{F,\,G\Big\}_{\rm gc} = \epsilon^{-1}\left(\frac{\partial F}{\partial\theta}\,\frac{\partial G}{\partial J} \;-\; \frac{\partial F}{\partial J}\,\frac{\partial G}{\partial\theta}\right) \;+\; \frac{{\bf B}^{*}}{B_{\|}^{**}}\cdot\left(\nabla^{*}F\,\frac{\partial G}{\partial p_{\|}} \;-\; \frac{\partial F}{\partial p_{\|}}\,\nabla^{*}G\right)$$
$$-\;\frac{\epsilon\,c\widehat{\sf b}^{*}}{e\,B_{\|}^{**}}\cdot\nabla^{*}F\times\nabla^{*}G, \tag{2.12}$$

where the modified gradient operator $\nabla^{*} \equiv \nabla + {\bf R}^{*}\partial/\partial\theta$ ensures gyrogauge-invariance. The derivation procedure of the guiding-center Poisson bracket (2.12) guarantees that it satisfies the standard Poisson-bracket properties, while the guiding-center Jacobian (2.6) can be used to write Eq. (2.12) in phase-space divergence form

$$\Big\{F,\,G\Big\}_{\rm gc} \;=\; \frac{1}{\mathcal{J}_{\rm gc}}\,\frac{\partial}{\partial Z^{\alpha}}\Big(\mathcal{J}_{\rm gc}\;F\;\{Z^{\alpha},\;G\}_{\rm gc}\Big). \tag{2.13}$$

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 (2.1) and the guiding-center Poisson bracket (2.12) as

$$\frac{d_{\rm gc}{\bf X}}{dt} = \left(\frac{p_{\|}}{m} + \frac{\partial\Psi}{\partial p_{\|}}\right)\,\frac{{\bf B}^{*}}{B_{\|}^{**}} \;+\; \frac{\epsilon\,c\widehat{\sf b}^{*}}{e\,B_{\|}^{**}}\times\nabla\Psi, \tag{2.14}$$

$$\frac{d_{\rm gc}p_{\|}}{dt} = -\,\frac{{\bf B}^{*}}{B_{\|}^{**}}\cdot\nabla\Psi, \tag{2.15}$$

$$\frac{d_{\rm gc}\theta}{dt} = \epsilon^{-1}\,\frac{\partial\Psi}{\partial J} \;+\; \frac{d_{\rm gc}{\bf X}}{dt}\cdot\left({\bf R} \;-\; \epsilon^{-1}\frac{\partial{\bf \Pi}}{\partial J}\right), \tag{2.16}$$

and

$$\frac{d_{\rm gc}J}{dt} \;=\; -\,\epsilon^{-1}\,\frac{\partial\Psi}{\partial\theta} \;\equiv\; 0, \tag{2.17}$$

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 (2.14)-(2.15) satisfy the guiding-center Liouville theorem

$$\nabla\cdot\left(B_{\|}^{**}\,\frac{d_{\rm gc}{\bf X}}{dt}\right) \;+\; \frac{\partial}{\partial p_{\|}}\left(B_{\|}^{**}\,\frac{d_{\rm gc}p_{\|}}{dt}\right) \;=\; 0, \tag{2.18}$$

which follows from the identities (2.11).

Lastly, it will be useful in what follows to expand Eqs. (2.14)-(2.16) in powers of ϵ as

$$\frac{d_{\rm gc}Z^{\alpha}}{dt} \;\equiv\; \sum_{n=0}^{\infty}\,\epsilon^{n}\,\frac{d_{n}^{*}Z^{\alpha}}{dt}, \tag{2.19}$$

where, up to second order in ϵ (without expanding $B_{\|}^{**}$), we find

$$\frac{d_0^*\mathbf{X}}{dt} = \frac{p_\|}{m}\,\frac{\mathbf{B}}{B_\|^{**}}, \tag{2.20}$$

$$\frac{d_1^*\mathbf{X}}{dt} = \frac{\partial\Psi_1}{\partial p_\|}\,\frac{\mathbf{B}}{B_\|^{**}} \;+\; \frac{c}{e\,B_\|^{**}}\left(\frac{p_\|^2}{m}\,\nabla\times\widehat{\mathsf{b}} + \widehat{\mathsf{b}}\times\nabla(J\Omega)\right), \tag{2.21}$$

$$\begin{aligned}\frac{d_2^*\mathbf{X}}{dt} &= \frac{\partial\Psi_2}{\partial p_\|}\,\frac{\mathbf{B}}{B_\|^{**}} \;+\; \frac{c}{e\,B_\|^{**}}\left[\frac{p_\|}{m}\,\nabla\times(\mathbf{\Pi}_1 - J\,\mathbf{R}) \;+\; \frac{\partial\mathbf{\Pi}_1}{\partial p_\|}\times\nabla(J\,\Omega)\right] \\ &\quad + \frac{c}{e\,B_\|^{**}}\left(p_\|\,\frac{\partial\Psi_1}{\partial p_\|}\,\nabla\times\widehat{\mathsf{b}} \;+\; \widehat{\mathsf{b}}\times\nabla\Psi_1\right),\end{aligned} \tag{2.22}$$

$$\frac{d_0^*p_\|}{dt} = -\,\frac{\mathbf{B}}{B_\|^{**}}\cdot\nabla(J\,\Omega) \;=\; J\,\Omega\;(\nabla\cdot\widehat{\mathsf{b}})\;\frac{B}{B_\|^{**}}, \tag{2.23}$$

$$\frac{d_1^*p_\|}{dt} = -\,\frac{cp_\|}{e\,B_\|^{**}}\,\nabla\times\widehat{\mathsf{b}}\cdot\nabla(J\,\Omega) \;-\; \frac{\mathbf{B}}{B_\|^{**}}\cdot\nabla\Psi_1, \tag{2.24}$$

$$\frac{d_2^*p_\|}{dt} = -\,\frac{c}{e\,B_\|^{**}}\left[p_\|\,\nabla\times\widehat{\mathsf{b}}\cdot\nabla\Psi_1 + \nabla\times(\mathbf{\Pi}_1 - J\,\mathbf{R})\cdot\nabla(J\,\Omega)\right] - \frac{\mathbf{B}}{B_\|^{**}}\cdot\nabla\Psi_2, \tag{2.25}$$

which satisfy the guiding-center Liouville theorem (2.18) separately:

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

at each order ϵ^n (for $n = 0, 1, 2, ...$). We will also need the expression

$$\frac{d_{\rm gc}\theta}{dt} = \epsilon^{-1}\left(\Omega + \epsilon\,\frac{\partial\Psi_1}{\partial J} + \epsilon^2\,\frac{\partial\Psi_2}{\partial J} + \cdots\right) + \frac{d_{\rm gc}\mathbf{X}}{dt}\cdot\left(\mathbf{R} - \frac{\partial\mathbf{\Pi}_1}{\partial J} - \epsilon\,\frac{\partial\mathbf{\Pi}_2}{\partial J} + \cdots\right), \tag{2.26}$$

where the first term ($\epsilon^{-1}\Omega$) is dominant while the remaining terms vanish in a uniform magnetic field.

The guiding-center Hamiltonian (2.1) and the guiding-center phase-space Lagrangian (2.3) are defined in terms of the scalar field Ψ and the vector field $\mathbf{\Pi}$. In a purely *Hamiltonian* representation, the vector field $\mathbf{\Pi} \equiv p_\|\,\widehat{\mathsf{b}}$ 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. Hence, in the Hamiltonian representation, the vector field $\widehat{\mathsf{b}}^*$ in Eq. (2.14) is $\widehat{\mathsf{b}}^* \equiv \partial\mathbf{\Pi}/\partial p_\| = \widehat{\mathsf{b}}$ while $\mathbf{R}^* \equiv \mathbf{R} - \partial\mathbf{\Pi}/\partial J = \mathbf{R}$ in Eq. (2.16). In a purely *symplectic* representation, on the other hand, the scalar field $\Psi \equiv J\,\Omega$ is independent of the parallel momentum $p_\|$, while the vector field $\mathbf{\Pi} = p_\|\,\widehat{\mathsf{b}} + \epsilon\,\mathbf{\Pi}_1 + \cdots$ contains all the correction terms associated with the nonuniformity of the magnetic field. Hence, the vector fields $\widehat{\mathsf{b}}^*$ and $\mathbf{R}^*$ are defined in terms of the expressions (2.8)-(2.9), respectively.

In the perturbation analysis presented below, it will be shown that a purely symplectic representation is impossible, i.e., $\Psi \neq J\,\Omega$ to all orders in ϵ. In standard guiding-center and gyrokinetic theories, we find $\Psi_1 \equiv 0$ and $\mathbf{\Pi}_1 \neq 0$ at first order, which will also be adopted in the present work.

3. Guiding-center phase-space Lagrangian: Lie-transform Derivation

The derivation of the guiding-center Hamiltonian (2.1) and the guiding-center phase-space Lagrangian (2.3) 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 $(\mathsf{G}_1, \mathsf{G}_2, \cdots)$:

$$Z^\alpha \;=\; z^\alpha \;+\; \epsilon\, G_1^\alpha \;+\; \epsilon^2 \left(G_2^\alpha + \frac{1}{2}\,\mathsf{G}_1\cdot\mathsf{d}G_1^\alpha\right) \;+\; \cdots, \tag{3.1}$$

and its inverse

$$z^\alpha \;=\; Z^\alpha \;-\; \epsilon\, G_1^\alpha \;-\; \epsilon^2 \left(G_2^\alpha - \frac{1}{2}\,\mathsf{G}_1\cdot\mathsf{d}G_1^\alpha\right) \;+\; \cdots. \tag{3.2}$$

The guiding-center Jacobian (2.6) associated with the phase-space transformation (3.1) is defined as

$$\begin{aligned}\mathcal{J}_{\rm gc} \equiv \mathcal{J}_0 \;-\; \frac{\partial}{\partial z^\alpha}\left[\mathcal{J}_0\left(\epsilon\, G_1^\alpha \;+\; \epsilon^2\, G_2^\alpha + \cdots\right) \;-\; \frac{\epsilon^2}{2}\, G_1^\alpha\, \frac{\partial}{\partial z^\beta}\left(\mathcal{J}_0\, G_1^\beta + \cdots\right) \;+\; \cdots\right] \\ = \mathcal{J}_0 \;+\; \epsilon\,\mathcal{J}_1 \;+\; \epsilon^2\,\mathcal{J}_2 \;+\; \cdots\end{aligned} \tag{3.3}$$

where $\mathcal{J}_0 \equiv e\,B/c$. Next, the effective guiding-center potential energy (2.2) is defined in terms of the guiding-center transformation as

$$\Psi_1 - \frac{p_\|}{m}\,\Pi_{1\|} \equiv -\,\Omega\left(G_1^J \;+\; J\,G_1^{\mathbf{x}}\boldsymbol{\cdot}\nabla\ln B\right) \;-\; \frac{p_\|}{m}\,\left(G_1^{p_\|} \;+\; \Pi_{1\|}\right), \tag{3.4}$$

$$\Psi_2 - \frac{p_\|}{m}\,\Pi_{2\|} \equiv -\,\Omega\left(G_2^J \;+\; J\,G_2^{\mathbf{x}}\boldsymbol{\cdot}\nabla\ln B\right) \;-\; \frac{p_\|}{m}\,\left(G_2^{p_\|} \;+\; \Pi_{2\|}\right) \;-\; \frac{1}{2}\,\mathsf{G}_1\cdot\mathsf{d}\Psi_1. \tag{3.5}$$

Beginning with the general relation between the old (particle) phase-space Lagrangian

$$\gamma \;\equiv\; \left(\frac{e}{\epsilon\, c}\,\mathbf{A} \;+\; \mathbf{p}\right)\boldsymbol{\cdot}\mathsf{d}\mathbf{x} \;=\; \epsilon^{-1}\,\gamma_0 \;+\; \gamma_1, \tag{3.6}$$

we derive the new (guiding-center) phase-space Lagrangian $\Gamma_{\rm gc}$:

$$\Gamma_{\rm gc} = \mathsf{T}_{\rm gc}^{-1}\gamma \;+\; \mathsf{d}S \;\equiv\; \epsilon^{-1}\left(\Gamma_0 \;+\; \epsilon\,\Gamma_1 \;+\; \epsilon^2\,\Gamma_2 \;+\; \cdots\right), \tag{3.7}$$

where each perturbation term $\Gamma_n \equiv \Gamma_{n\alpha}\,\mathsf{d}Z^\alpha + \mathsf{d}S_n$ is expressed in terms of the symplectic components $\Gamma_{n\alpha}$ and the nth-order component of the phase-space gauge function $S \equiv S_1 + \epsilon\, S_2 + \cdots$. In Eq. (3.7), the *push-forward* operator $\mathsf{T}_{\rm gc}^{-1} \equiv \cdots\exp(-\,\epsilon^2\pounds_2)\,\exp(-\,\epsilon\pounds_1)$ is defined in terms of the product of Lie-transforms $\exp(-\epsilon^n\,\pounds_n)$, where the nth-order Lie derivative $\pounds_n$ is generated by the nth-order vector field G_n. According to Cartan's homotopy formula, the Lie derivative $\pounds_G$ of a one-form γ yields the one-form

$$\pounds_G\gamma \equiv \iota_G\cdot\mathsf{d}\gamma \;+\; \mathsf{d}(\iota_G\cdot\gamma) \;=\; G^\alpha\,\omega_{\alpha\beta}\,\mathsf{d}z^\beta \;+\; \mathsf{d}\left(G^\alpha\,\gamma_\alpha\right). \tag{3.8}$$

Note that, according to this formula, the exterior derivative d and the Lie derivative $\pounds_G$ commute, i.e., $\pounds_G(\mathsf{d}\gamma) = \mathsf{d}(\pounds_G\gamma)$. Furthermore, an arbitrary exact exterior derivative $\mathsf{d}S$ can be added to the push-forward $\mathsf{T}_{\rm gc}^{-1}\gamma$ in Eq. (3.7) without affecting the guiding-center two-form

$$\boldsymbol{\omega}_{\rm gc} \equiv \mathsf{d}\Gamma_{\rm gc} \;=\; \mathsf{d}\left(\mathsf{T}_{\rm gc}^{-1}\gamma\right) \;+\; \mathsf{d}^2 S \;=\; \mathsf{T}_{\rm gc}^{-1}\left(\mathsf{d}\gamma\right) \;=\; \mathsf{T}_{\rm gc}^{-1}\boldsymbol{\omega}, \tag{3.9}$$

since d^2 for any k-form vanishes and the push-forward $\mathsf{T}_{\rm gc}^{-1}$ commutes with d (because all functions of Lie derivatives do).

When the push-forward $\mathsf{T}_{\rm gc}^{-1}$ and the phase-space gauge function S are expanded in powers of ϵ in Eq. (3.7), we obtain the zeroth-order equation

$$\Gamma_0 \;=\; \gamma_0 \;\equiv\; \frac{e}{c}\,\mathbf{A}(\mathbf{X})\cdot\mathsf{d}\mathbf{X}, \tag{3.10}$$

the first-order equation

$$\Gamma_1 \;=\; \gamma_1 \;-\; \pounds_1\,\gamma_0 \;+\; \mathsf{d}S_1 \;\equiv\; \gamma_1 \;-\; \iota_1\cdot\boldsymbol{\omega}_0 \;+\; \mathsf{d}\sigma_1, \tag{3.11}$$

the second-order equation

$$\begin{aligned}\Gamma_2 =& -\,\pounds_2\,\gamma_0 \;-\; \pounds_1\,\gamma_1 \;+\; \frac{1}{2}\,\pounds_1^2\,\gamma_0 \;+\; \mathsf{d}S_2\\ \equiv& -\,\iota_2\cdot\omega_0 \;-\; \frac{1}{2}\,\iota_1\cdot\Big(\boldsymbol{\omega}_1 \;+\; \boldsymbol{\omega}_{\rm gc1}\Big) \;+\; \mathsf{d}\sigma_2,\end{aligned} \tag{3.12}$$

the third-order equation

$$\begin{aligned}\Gamma_3 =& -\,\pounds_3\,\gamma_0 \;-\; \pounds_2\,\gamma_1 \;+\; \frac{1}{2}\,\pounds_1^2\,\gamma_1 \;+\; \pounds_2\pounds_1\,\gamma_0 \;-\; \frac{1}{6}\,\pounds_1^3\,\gamma_0 \;+\; \mathsf{d}S_3\\ \equiv& -\iota_3\cdot\boldsymbol{\omega}_0 \;-\; \iota_2\cdot\boldsymbol{\omega}_{\rm gc1} \;+\; \frac{\iota_1}{3}\cdot\mathsf{d}\left(\iota_1\cdot\boldsymbol{\omega}_1 + \frac{\iota_1}{2}\cdot\boldsymbol{\omega}_{\rm gc1}\right) \;+\; \mathsf{d}\sigma_3,\end{aligned} \tag{3.13}$$

and the fourth-order equation

$$\begin{aligned}\Gamma_4 =& -\,\pounds_4\,\gamma_0 \;+\; \pounds_3\,(\pounds_1\gamma_0 \;-\; \gamma_1) \;+\; \pounds_2\left(\pounds_1\gamma_1 \;-\; \frac{1}{2}\,\pounds_1^2\gamma_0 \;+\; \frac{1}{2}\,\pounds_2\gamma_0\right)\\ &-\,\frac{1}{6}\,\pounds_1^3\left(\gamma_1 \;-\; \frac{1}{4}\,\pounds_1\gamma_0\right) \;+\; \mathsf{d}S_4\\ \equiv& -\,\iota_4\cdot\boldsymbol{\omega}_0 \;-\; \iota_3\cdot\boldsymbol{\omega}_{\rm gc1} \;-\; \frac{\iota_2}{2}\cdot\left[\boldsymbol{\omega}_{\rm gc2} \;-\; \frac{1}{2}\,\mathsf{d}\left(\iota_1\cdot\boldsymbol{\omega}_1 \;+\; \iota_1\cdot\boldsymbol{\omega}_{\rm gc1}\right)\right]\\ &-\,\frac{\iota_1}{8}\cdot\mathsf{d}\left[\iota_1\cdot\mathsf{d}\left(\iota_1\cdot\boldsymbol{\omega}_1 \;+\; \frac{\iota_1}{3}\cdot\boldsymbol{\omega}_{\rm gc1}\right)\right] \;+\; \mathsf{d}\sigma_4,\end{aligned} \tag{3.14}$$

where $\iota_n\cdot\boldsymbol{\omega}_k = G_n^\alpha\,\omega_{k\alpha\beta}\;\mathsf{d}z^\beta$ and, since $\pounds_n\gamma_k = \iota_n\cdot\boldsymbol{\omega}_k + \mathsf{d}(\iota_n\cdot\gamma_k)$, we have redefined the phase-space gauge functions $S_n \to \sigma_n$ by absorbing all exact exterior derivatives: $\mathsf{d}(\cdots) + \mathsf{d}S_n \equiv \mathsf{d}\sigma_n$ (i.e., $\sigma_1 \equiv S_1 - \iota_1\cdot\gamma_0$). The phase-space gauge functions σ_n in Eqs. (3.11)-(3.14) are generally considered to be gyroangle-dependent functions (i.e., $\langle\sigma_n\rangle = 0$) but it is not a strict requirement. Note also that we use results obtained at lower orders to simplify expressions at each higher order (i.e., at second order, we use $\pounds_1\gamma_1 - \frac{1}{2}\,\pounds_1^2\gamma_0 = \frac{1}{2}\,\pounds_1\gamma_1 + \frac{1}{2}\,\pounds_1\Gamma_1$).

In Eqs. (3.11)-(3.13), we need to evaluate the contractions $\iota_n\cdot\boldsymbol{\omega}_0$ generated by the vector fields $(\mathsf{G}_1, \mathsf{G}_2, \cdots)$ on the zeroth-order two-form:

$$\boldsymbol{\omega}_0 = \mathsf{d}\gamma_0 \;=\; \frac{e}{c}\,\frac{\partial A_j}{\partial x^i}\,\mathsf{d}X^i \;\wedge\; \mathsf{d}X^j \;\equiv\; \frac{1}{2}\,\omega_{0\,ij}\,\mathsf{d}X^i \;\wedge\; \mathsf{d}X^j, \tag{3.15}$$

where the magnetic field is $\mathbf{B} \equiv \nabla\times\mathbf{A}$. Using the contraction formula (3.8), we obtain the n^{th}-order expression

$$\iota_n\cdot\boldsymbol{\omega}_0 \;=\; \frac{e}{c}\,\mathbf{B}\times G_n^{\mathbf{x}}\cdot\mathsf{d}\mathbf{X}, \tag{3.16}$$

where $G_n^{\mathbf{x}}$ denote the spatial components of the nth-order generating vector field G_n.

Similarly, in Eqs. (3.12)-(3.13), we need to evaluate the contractions $\iota_n\cdot\boldsymbol{\omega}_1$ generated by the vector fields $(\mathsf{G}_1, \mathsf{G}_2, \cdots)$ on the first-order two-form $\boldsymbol{\omega}_1 = \mathsf{d}\gamma_1$. When evaluated explicitly, we obtain the $(n+1)^{\rm th}$-order expression

$$\iota_n\cdot\boldsymbol{\omega}_1 \equiv D_n(p_\parallel\,\widehat{\mathsf{b}} + \mathbf{p}_\perp)\cdot\mathsf{d}\mathbf{X} \;-\; G_n^{\mathbf{x}}\cdot\left(\widehat{\mathsf{b}}\;\mathsf{d}p_\parallel + \frac{\partial\mathbf{p}_\perp}{\partial J}\;\mathsf{d}J + \frac{\partial\mathbf{p}_\perp}{\partial\theta}\;\mathsf{d}\theta\right). \tag{3.17}$$

Here, the spatial components are expressed in terms of the operator $D_n(\cdots)$ defined as

$$D_n(\cdots) \equiv \left(G_n^{p_\|} \frac{\partial}{\partial p_\|} + G_n^J \frac{\partial}{\partial J} + G_n^\theta \frac{\partial}{\partial \theta} \right)(\cdots) \;-\; G_n^{\mathbf{x}} \times \nabla\times(\cdots). \tag{3.18}$$

4. First-order Perturbation Analysis

We begin our perturbation analysis by considering the first-order guiding-center symplectic one-form (3.11), which is now explicitly written as

$$\begin{aligned} \Gamma_1 &= \left(p_\| \,\widehat{\mathsf{b}} \;+\; \mathbf{p}_\perp \right) \cdot \mathsf{d}\mathbf{X} \;-\; \frac{e}{c}\,\mathbf{B}\times G_1^{\mathbf{x}}\cdot \mathsf{d}\mathbf{X} \;+\; \mathsf{d}\sigma_1 \\ &= p_\|\,\widehat{\mathsf{b}}\cdot\mathsf{d}\mathbf{X} \;+\; \left(\mathbf{p}_\perp \;-\; \frac{e}{c}\,\mathbf{B}\times G_1^{\mathbf{x}} \right)\cdot\mathsf{d}\mathbf{X} \;+\; \mathsf{d}\sigma_1 \qquad (4.1) \\ &\equiv p_\|\,\widehat{\mathsf{b}}\cdot\mathsf{d}\mathbf{X}, \qquad (4.2) \end{aligned}$$

where we have separated the terms that are independent and dependent on the gyroangle θ. It is immediately clear that the first-order phase-space gauge function σ_1 is not needed to remove the gyroangle dependence on the right side of Eq. (4.1), and thus we set $\sigma_1 \equiv 0$.

The spatial components $G_1^{\mathbf{x}}$ of the first-order generating vector field G_1 is determined by the condition

$$\mathbf{p}_\perp \;-\; (e/c)\,\mathbf{B}\times G_1^{\mathbf{x}} \;\equiv\; 0,$$

which removes the gyroangle dependence in the first-order phase-space Lagrangian (4.1). This condition can easily be solved as

$$G_1^{\mathbf{x}} \;=\; \left(\widehat{\mathsf{b}}\cdot G_1^{\mathbf{x}} \right)\,\widehat{\mathsf{b}} \;-\; \frac{c\widehat{\mathsf{b}}}{eB}\times\mathbf{p}_\perp \;\equiv\; G_{1\|}^{\mathbf{x}}\,\widehat{\mathsf{b}} \;-\; \boldsymbol{\rho}_0, \tag{4.3}$$

where $G_{1\|}^{\mathbf{x}} \equiv \widehat{\mathsf{b}}\cdot G_1^{\mathbf{x}}$ denotes the parallel component of $G_1^{\mathbf{x}}$ (undetermined at this order).

With $\sigma_1 \equiv 0$ and $G_1^{\mathbf{x}}$ defined by Eq. (4.3), the resulting first-order guiding-center phase-space Lagrangian is given Eq. (4.2), where all spatially-dependent fields are now evaluated at the guiding-center position $\mathbf{X}$. Hence, we obtain the nth-order contraction

$$\iota_n \cdot \omega_{\rm gc1} \;\equiv\; D_n(p_\|\,\widehat{\mathsf{b}})\cdot\mathsf{d}\mathbf{X} \;-\; G_{n\|}^{\mathbf{x}}\;\mathsf{d}p_\|, \tag{4.4}$$

where $G_{n\|}^{\mathbf{x}} \equiv \widehat{\mathsf{b}}\cdot G_n^{\mathbf{x}}$ denotes the parallel component of $G_n^{\mathbf{x}}$, and the spatial components in Eq. (4.4) are

$$D_n(p_\|\,\widehat{\mathsf{b}}) = \left(G_n^{p_\|} \;-\; p_\|\,\boldsymbol{\kappa}\cdot G_n^{\mathbf{x}} \right)\,\widehat{\mathsf{b}} \;+\; p_\|\;\left(\tau\,\widehat{\mathsf{b}}\times G_n^{\mathbf{x}} \;+\; G_{n\|}^{\mathbf{x}}\;\boldsymbol{\kappa} \right). \tag{4.5}$$

5. Second-order Perturbation Analysis

We now proceed with the second-order guiding-center symplectic one-form (3.12), now explicitly expressed as

$$\begin{aligned} \Gamma_2 &= -\;\left[\frac{e}{c}\mathbf{B}\times G_2^{\mathbf{x}} \;+\; D_1(\mathbf{P}_2) \right]\cdot\mathsf{d}\mathbf{X} \;+\; \frac{1}{2}\,G_1^{\mathbf{x}}\cdot\left(\frac{\partial\mathbf{p}_\perp}{\partial J}\,\mathsf{d}J + \frac{\partial\mathbf{p}_\perp}{\partial\theta}\,\mathsf{d}\theta \right) \\ &= -\;\left[\frac{e}{c}\mathbf{B}\times G_2^{\mathbf{x}} \;+\; D_1(\mathbf{P}_2) \right]\cdot\mathsf{d}\mathbf{X} \;+\; J\;\mathsf{d}\theta \qquad (5.1) \\ &\equiv \boldsymbol{\Pi}_1\cdot\mathsf{d}\mathbf{X} \;+\; J\;\left(\mathsf{d}\theta \;-\; \mathbf{R}\cdot\mathsf{d}\mathbf{X} \right), \qquad (5.2) \end{aligned}$$

where

$$\mathbf{P}_2 \;\equiv\; p_\|\,\widehat{\mathsf{b}} + \frac{1}{2}\,\mathbf{p}_\perp, \tag{5.3}$$

and we used $\sigma_2 \equiv 0$ with $G_1^{\mathbf{x}}\cdot\partial\mathbf{p}_\perp/\partial J = 0$ and $G_1^{\mathbf{x}}\cdot\partial\mathbf{p}_\perp/\partial\theta = 2\,J$. Since $G_{1\|}^{\mathbf{x}} \equiv -\,\partial\sigma_2/\partial p_\| \equiv 0$, the spatial component of G_1 is now exactly

$$G_1^{\mathbf{x}} \;=\; -\,\boldsymbol{\rho}_0, \tag{5.4}$$

i.e., to lowest order, the displacement from the particle position $\mathbf{x}$ to the guiding-center position $\mathbf{X}$ is perpendicular to $\mathbf{B}$.

Using Eqs. (3.18) and (4.5) for $n = 1$, with Eq. (5.3), we find

$$\begin{aligned} D_1(\mathbf{P}_2) = {} & \left(G_1^{p_\|} \;+\; p_\|\,\boldsymbol{\rho}_0\cdot\boldsymbol{\kappa}\right)\,\widehat{\mathsf{b}} \;+\; p_\|\,\tau\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} \;+\; J\left[\mathbf{R} \;-\; \left(\frac{\tau}{2} \;+\; \alpha_1\right)\widehat{\mathsf{b}}\right] \\ & +\;\frac{1}{2}\,\left(G_1^J \;-\; J\,\boldsymbol{\rho}_0\cdot\nabla\ln B\right)\,\frac{\partial\mathbf{p}_\perp}{\partial J} \;+\; \frac{1}{2}\,\left(G_1^\theta \;+\; \boldsymbol{\rho}_0\cdot\mathbf{R}\right)\,\frac{\partial\mathbf{p}_\perp}{\partial\theta}, \end{aligned} \tag{5.5}$$

where $\alpha_1 \equiv \mathsf{a}_1 : \nabla\widehat{\mathsf{b}}$ is defined in App. A. We note that $\mathbf{R}$ appears in Eq. (5.2) in order to satisfy the property of gyrogauge invariance. With this choice, we obtain the vector equation

$$J\,\mathbf{R} \;-\; \boldsymbol{\Pi}_1 \;\equiv\; \frac{e}{c}\,\mathbf{B}\times G_2^{\mathbf{x}} \;+\; D_1(\mathbf{P}_2). \tag{5.6}$$

From the parallel components of Eqs. (5.5)-(5.6), we obtain the first-order component

$$G_1^{p_\|} \;=\; -\,p_\|\,\boldsymbol{\rho}_0\cdot\boldsymbol{\kappa} \;+\; J\left(\frac{\tau}{2} \;+\; \alpha_1\right) \;-\; \Pi_{1\|}, \tag{5.7}$$

where $\Pi_{1\|} \equiv \widehat{\mathsf{b}}\cdot\boldsymbol{\Pi}_1$. By using the definition (3.4), on the other hand, we obtain the first-order component

$$\begin{aligned} G_1^J & \equiv J\,\boldsymbol{\rho}_0\cdot\nabla\ln B \;-\; \varrho_\|\,G_1^{p_\|} \;-\; \Psi_1/\Omega \\ & = \boldsymbol{\rho}_0\cdot\left(J\,\nabla\ln B \;+\; \frac{p_\|^2}{m\Omega}\,\boldsymbol{\kappa}\right) \;-\; J\,\varrho_\|\,\left(\frac{\tau}{2} \;+\; \alpha_1\right) \;+\; \left(\varrho_\|\,\Pi_{1\|} - \frac{\Psi_1}{\Omega}\right), \end{aligned} \tag{5.8}$$

which yields the first-order guiding-center Hamiltonian constraint

$$\frac{p_\|}{m}\,\Pi_{1\|} \;-\; \Psi_1 \;=\; \Omega\left(\langle G_1^J\rangle \;-\; \frac{1}{2}\,J\,\varrho_\|\,\tau\right). \tag{5.9}$$

In the next Section, we will discuss how $\Pi_{1\|}$ and Ψ_1 may be chosen once $\langle G_1^J\rangle$ is known.

Lastly, from the perpendicular components of Eq. (5.6), we find

$$\begin{aligned} G_2^{\mathbf{x}} = {} & G_{2\|}^{\mathbf{x}}\,\widehat{\mathsf{b}} \;+\; \boldsymbol{\rho}_0\,(\varrho_\|\,\tau) \;+\; \frac{1}{2}\left(G_1^J - \;J\,\boldsymbol{\rho}_0\cdot\nabla\ln B\right)\frac{\partial\boldsymbol{\rho}_0}{\partial J} \\ & +\;\frac{1}{2}\,(G_1^\theta + \boldsymbol{\rho}_0\cdot\mathbf{R})\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} \;-\; \boldsymbol{\Pi}_1\times\frac{\widehat{\mathsf{b}}}{m\Omega}, \end{aligned} \tag{5.10}$$

where $G_{2\|}^{\mathbf{x}} \equiv \widehat{\mathsf{b}}\cdot G_2^{\mathbf{x}}$ denotes the parallel component of $G_2^{\mathbf{x}}$.

6. Third-order Perturbation Analysis

The third-order guiding-center symplectic one-form (3.13) is explicitly given in terms of the spatial components

$$\Gamma_{3\mathbf{x}} = D_1^2(\mathbf{P}_3) \;-\; \frac{e}{c}\,\mathbf{B}\times G_3^{\mathbf{x}} \;-\; D_2\left(p_\|\,\widehat{\mathsf{b}}\right) \;+\; \nabla\sigma_3 \;\equiv\; \boldsymbol{\Pi}_2, \tag{6.1}$$

and the momentum components

$$\Gamma_{3\mathbf{p}} \equiv \left[G_{2\parallel}^{\mathbf{x}} \;+\; \frac{\partial D_1(\mathbf{P}_3)}{\partial p_\parallel}\cdot\boldsymbol{\rho}_0 \;+\; \frac{\partial\sigma_3}{\partial p_\parallel}\right] \mathsf{d}p_\parallel + \left[\frac{2}{3}\,G_1^\theta + \frac{\partial D_1(\mathbf{P}_3)}{\partial J}\cdot\boldsymbol{\rho}_0 + \frac{\partial\sigma_3}{\partial J}\right] \mathsf{d}J$$
$$+ \left[-\,\frac{2}{3}\,G_1^J + \frac{\partial D_1(\mathbf{P}_3)}{\partial\theta}\cdot\boldsymbol{\rho}_0 + \frac{\partial\sigma_3}{\partial\theta}\right] \mathsf{d}\theta \;\equiv\; 0, \tag{6.2}$$

where

$$\mathbf{P}_3 \;\equiv\; \frac{1}{2}\,p_\parallel\widehat{\mathsf{b}} + \frac{1}{3}\,\mathbf{p}_\perp. \tag{6.3}$$

In Eqs. (6.1)-(6.2), we find

$$D_1(\mathbf{P}_3) = \frac{1}{2}\,G_1^{p_\parallel}\,\widehat{\mathsf{b}} \;+\; \frac{1}{3}\left(G_1^J\,\frac{\partial\mathbf{p}_\perp}{\partial J} + G_1^\theta\,\frac{\partial\mathbf{p}_\perp}{\partial\theta}\right) \;+\; \boldsymbol{\rho}_0\times\nabla\times\mathbf{P}_3, \tag{6.4}$$

$$D_1^2(\mathbf{P}_3) \equiv \frac{1}{2}\,D_1^2(p_\parallel\widehat{\mathsf{b}}) + \frac{1}{3}\,D_1^2(\mathbf{p}_\perp), \tag{6.5}$$

and

$$D_2(p_\parallel\,\widehat{\mathsf{b}}) = \left(G_2^{p_\parallel} \;-\; p_\parallel\,\boldsymbol{\kappa}\cdot G_2^{\mathbf{x}}\right)\,\widehat{\mathsf{b}} \;+\; p_\parallel\;\left(\tau\,\widehat{\mathsf{b}}\times G_2^{\mathbf{x}} \;+\; G_{2\parallel}^{\mathbf{x}}\,\boldsymbol{\kappa}\right). \tag{6.6}$$

6.1. *Momentum components*

If we define the new gauge function

$$\overline{\sigma}_3 \;\equiv\; \sigma_3 \;+\; D_1(\mathbf{P}_3)\cdot\boldsymbol{\rho}_0 \;=\; \sigma_3 \;-\; \frac{2}{3}\;J\,G_1^\theta, \tag{6.7}$$

where the last expression follows from Eq. (6.4), the momentum components (6.2) become

$$\Gamma_{3\mathbf{p}} = \left(G_{2\parallel}^{\mathbf{x}} \;+\; \frac{\partial\overline{\sigma}_3}{\partial p_\parallel}\right)\,\mathsf{d}p_\parallel \;+\; \left(G_1^\theta \;+\; \frac{\partial\overline{\sigma}_3}{\partial J}\right)\,\mathsf{d}J$$
$$+ \left[\frac{\partial\overline{\overline{\sigma}}_3}{\partial\theta} \;-\; \left(G_1^J \;+\; J\;\varrho_\parallel\tau\right)\right]\,\mathsf{d}\theta, \tag{6.8}$$

where we introduced yet another gauge function

$$\overline{\overline{\sigma}}_3 \;\equiv\; \overline{\sigma}_3 \;-\; \frac{1}{3}\left(2\,J\,\boldsymbol{\rho}_0\cdot\mathbf{R} \;+\; J\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\nabla\ln B\right) \tag{6.9}$$

in the θ-component. By requiring that the momentum components (6.8) vanish, $\Gamma_{3\mathbf{p}} \equiv 0$, we obtain the definitions

$$G_1^J \equiv -\,J\;\varrho_\parallel\tau \;+\; \frac{\partial\overline{\overline{\sigma}}_3}{\partial\theta}, \tag{6.10}$$

$$G_{2\parallel}^{\mathbf{x}} \equiv -\,\frac{\partial\overline{\sigma}_3}{\partial p_\parallel}, \tag{6.11}$$

$$G_1^\theta \equiv -\,\frac{\partial\overline{\sigma}_3}{\partial J}. \tag{6.12}$$

From Eq. (6.10), we immediately conclude that $\langle G_1^J\rangle$ must be defined as

$$\langle G_1^J\rangle \;\equiv\; -\,J\;\varrho_\parallel\tau. \tag{6.13}$$

By comparing Eq. (5.9) with Eq. (6.13), we obtain

$$\frac{p_\parallel}{m}\,\Pi_{1\parallel} \;-\; \Psi_1 \;\equiv\; -\,J\,\Omega\;\left(\frac{1}{2}\;\varrho_\parallel\;\tau\right). \tag{6.14}$$

One possible choice for $(\Pi_{1\|}, \Psi_1)$ 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. (2.21). We note here that, since the right side of Eq. (6.14) is linear in $p_\|$, we may choose $\Psi_1 \equiv 0$ without making $\Pi_{1\|}$ singular. In accordance with standard guiding-center Hamiltonian theory, we therefore choose

$$\left.\begin{array}{rcl} \Psi_1 & \equiv & 0 \\ \\ \Pi_{1\|} & \equiv & -\,\frac{1}{2}\,J\,\tau \end{array}\right\}, \tag{6.15}$$

so that Eqs. (5.7)-(5.8) become

$$G_1^{p_\|} = -\,p_\|\;\boldsymbol{\rho}_0\cdot\boldsymbol{\kappa} \;+\; J\,(\tau \;+\; \alpha_1)\,, \tag{6.16}$$

$$G_1^J = \boldsymbol{\rho}_0\cdot\left(J\,\nabla\ln B + \frac{p_\|^2\,\boldsymbol{\kappa}}{m\Omega}\right) - J\,\varrho_\|\,(\tau + \alpha_1). \tag{6.17}$$

Using Eq. (6.17), Eq. (6.10) yields a differential equation for $\overline{\overline{\sigma}}_3$:

$$\frac{\partial\overline{\overline{\sigma}}_3}{\partial\theta} \;=\; \boldsymbol{\rho}_0\cdot\left(J\,\nabla\ln B + \frac{p_\|^2}{m\,\Omega}\,\boldsymbol{\kappa}\right) - J\;\varrho_\|\,\alpha_1,$$

whose solution is

$$\overline{\overline{\sigma}}_3 = -\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\left(J\,\nabla\ln B + \frac{p_\|^2}{m\,\Omega}\,\boldsymbol{\kappa}\right) - J\;\varrho_\|\,\alpha_2, \tag{6.18}$$

where we used $\alpha_1 \equiv \partial\alpha_2/\partial\theta$ (see App. A). Next, we use Eq. (6.9) to obtain

$$\overline{\sigma}_3 = \frac{2}{3}\,J\left(\boldsymbol{\rho}_0\cdot\mathbf{R} \;-\; \frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\nabla\ln B\right) \;-\; \varrho_\|\left(p_\|\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\boldsymbol{\kappa} \;+\; J\,\alpha_2\right). \tag{6.19}$$

from which we obtain the remaining components (6.11)-(6.12):

$$G_{2\|}^{\mathbf{x}} = 2\;\varrho_\|\;\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\boldsymbol{\kappa} \;+\; \frac{J\,\alpha_2}{m\Omega}, \tag{6.20}$$

$$G_1^\theta = -\,\boldsymbol{\rho}_0\cdot\mathbf{R} \;+\; \varrho_\|\,\alpha_2 \;+\; \frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\left(\nabla\ln B \;+\; \frac{p_\|^2\,\boldsymbol{\kappa}}{2\,m\;J\Omega}\right). \tag{6.21}$$

By combining Eqs. (6.19) and (6.21) into Eq. (6.7), we also obtain the expression for σ_3:

$$\sigma_3 \;=\; \overline{\sigma}_3 \;+\; \frac{2J}{3}\;G_1^\theta \;\equiv\; -\,\frac{1}{3}\,p_\|\;G_{2\|}^{\mathbf{x}}, \tag{6.22}$$

where $G_{2\|}^{\mathbf{x}}$ is expressed in Eq. (6.20). Lastly, the second-order spatial component is now explicitly expressed as

$$\begin{aligned} G_2^{\mathbf{x}} = {} & \left(2\,\varrho_\|\;\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\boldsymbol{\kappa} \;+\; \frac{J\,\alpha_2}{m\Omega}\right)\widehat{\mathsf{b}} \;+\; \frac{1}{2}\left[\frac{p_\|^2}{m\Omega}\,(\boldsymbol{\rho}_0\cdot\boldsymbol{\kappa}) \;+\; J\,\varrho_\|\;(3\tau - \alpha_1)\right]\frac{\partial\boldsymbol{\rho}_0}{\partial J} \\ & +\; \frac{1}{2}\left[\varrho_\|\,\alpha_2 \;+\; \frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\left(\nabla\ln B \;+\; \frac{p_\|^2\,\boldsymbol{\kappa}}{2m\Omega\,J}\right)\right]\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} \;-\; \boldsymbol{\Pi}_1\times\frac{\widehat{\mathsf{b}}}{m\Omega}, \end{aligned} \tag{6.23}$$

from which we obtain the gyroangle-averaged expression

$$\langle G_2^{\mathbf{x}}\rangle \;=\; -\,\boldsymbol{\Pi}_1\times\frac{\widehat{\mathsf{b}}}{m\Omega} \;+\; \frac{1}{2}\left(\frac{J}{m\Omega}\;\nabla_\perp\ln B \;+\; \varrho_\|^2\;\boldsymbol{\kappa}\right). \tag{6.24}$$

6.2. *Spatial components*

The remaining components of the third-order one-form (6.1) are $\Gamma_{3\mathbf{x}} \equiv \boldsymbol{\Pi}_2$, where

$$\boldsymbol{\Pi}_2 = -\,\frac{e}{c}\,\mathbf{B}\times\left[G_3^{\mathbf{x}} \;-\; \varrho_\parallel\,\left(\tau\,G_{2\perp}^{\mathbf{x}} \;+\; G_{2\parallel}^{\mathbf{x}}\,\widehat{\mathsf{b}}\times\boldsymbol{\kappa}\right)\right] \\ -\;\left(G_2^{p_\parallel} - p_\parallel\,G_2^{\mathbf{x}}\cdot\boldsymbol{\kappa}\right)\widehat{\mathsf{b}} + D_1^2(\mathbf{P}_3) + \nabla\sigma_3, \tag{6.25}$$

which is now used to determine the components $G_2^{p_\parallel}$ and $G_{3\perp}^{\mathbf{x}}$.

The parallel spatial component of Eq. (6.25) yields the expression for $G_2^{p_\parallel}$:

$$G_2^{p_\parallel} = p_\parallel\;\boldsymbol{\kappa}\cdot G_2^{\mathbf{x}} \;+\; \widehat{\mathsf{b}}\cdot\left[D_1^2(\mathbf{P}_3) + \nabla\sigma_3 - \boldsymbol{\Pi}_2\right], \tag{6.26}$$

where σ_3 is defined in Eq. (6.22), and

$$\langle G_2^{p_\parallel}\rangle \;=\; -\;\varrho_\parallel\;\widehat{\mathsf{b}}\times\boldsymbol{\kappa}\cdot\boldsymbol{\Pi}_1 \;+\; \varrho_\parallel\;\boldsymbol{\kappa}\cdot\left(J\,\nabla\ln B \;+\; \frac{p_\parallel^2\boldsymbol{\kappa}}{m\Omega}\right) - \Pi_{2\parallel} \;+\; \widehat{\mathsf{b}}\cdot\left\langle D_1^2(\mathbf{P}_3)\right\rangle, \tag{6.27}$$

where $\Pi_{2\parallel} \equiv \widehat{\mathsf{b}}\cdot\boldsymbol{\Pi}_2$ and App. B gives the expression

$$\widehat{\mathsf{b}}\cdot\left\langle D_1^2(\mathbf{P}_3)\right\rangle \;=\; -\;J\;\varrho_\parallel\;\left(\frac{1}{2}\,\tau^2 \;-\; \langle\alpha_1^2\rangle\right). \tag{6.28}$$

With $G_2^{\mathbf{x}}$ and $G_2^{p_\parallel}$ given by Eqs. (6.23) and (6.26), G_2^J is now obtained from the definition (3.5):

$$G_2^J \equiv -\;J\,G_2^{\mathbf{x}}\cdot\nabla\ln B \;-\; \varrho_\parallel\;G_2^{p_\parallel} \;-\; \Psi_2/\Omega \tag{6.29}$$
$$= -\,G_2^{\mathbf{x}}\cdot\left(J\,\nabla\ln B \;+\; \frac{p_\parallel^2\,\boldsymbol{\kappa}}{m\,\Omega}\right) \;-\; \varrho_\parallel\widehat{\mathsf{b}}\cdot\left[D_1^2(\mathbf{P}_3) + \nabla\sigma_3\right] \;-\; \frac{1}{\Omega}\left(\Psi_2 \;-\; \frac{p_\parallel}{m}\,\Pi_{2\parallel}\right),$$

where we used the first-order choice (6.15): $\Psi_1 \equiv 0$. The gyroangle-averaged contribution of Eq. (6.29) yields

$$\left\langle G_2^J\right\rangle = -\;\langle G_2^{\mathbf{x}}\rangle\cdot\left(J\,\nabla\ln B \;+\; \frac{p_\parallel^2}{m\Omega}\,\boldsymbol{\kappa}\right) \;-\; \varrho_\parallel\,\widehat{\mathsf{b}}\cdot\left\langle D_1^2(\mathbf{P}_3)\right\rangle \;-\; \frac{1}{\Omega}\left(\Psi_2 \;-\; \frac{p_\parallel}{m}\,\Pi_{2\parallel}\right)$$
$$= \varrho_\parallel\,\Pi_{2\parallel} \;-\; \frac{1}{\Omega}\left(\Psi_2 \;+\; \frac{m}{2}\,|\mathbf{v}_{\rm gc}|^2 \;-\; \boldsymbol{\Pi}_1\cdot\mathbf{v}_{\rm gc}\right) \;+\; J\;\varrho_\parallel^2\left(\frac{1}{2}\,\tau^2 \;-\; \langle\alpha_1^2\rangle\right), \tag{6.30}$$

or the second-order guiding-center Hamiltonian constraint:

$$\frac{p_\parallel}{m}\,\Pi_{2\parallel} \;-\; \Psi_2 \;=\; \Omega\;\left[\langle G_2^J\rangle \;-\; J\;\varrho_\parallel^2\left(\frac{1}{2}\,\tau^2 \;-\; \langle\alpha_1^2\rangle\right)\right] \;+\; \frac{m}{2}\,|\mathbf{v}_{\rm gc}|^2 \;-\; \boldsymbol{\Pi}_1\cdot\mathbf{v}_{\rm gc}, \tag{6.31}$$

where $\langle G_2^J\rangle$ will be calculated at fourth order in the Lie-transform perturbation analysis, and the lowest-order guiding-center drift velocity is defined as

$$\mathbf{v}_{\rm gc} \;\equiv\; \frac{\widehat{\mathsf{b}}}{m}\times\left(J\,\nabla\ln B + \frac{p_\parallel^2}{m\Omega}\,\boldsymbol{\kappa}\right). \tag{6.32}$$

In the next Section, we will derive another expression for the gyroangle-averaged component $\langle G_2^J\rangle$.

Lastly, the perpendicular spatial components of Eq. (6.25), on the other hand, yields the expression for $G_3^{\mathbf{x}}$:

$$G_3^{\mathbf{x}} = G_{3\|}^{\mathbf{x}}\,\widehat{\mathsf{b}} \;+\; G_{2\|}^{\mathbf{x}}\,\left(\varrho_\|\,\nabla\times\widehat{\mathsf{b}}\right) \;-\; G_2^{\mathbf{x}}\,\left(\varrho_\|\,\tau\right)$$
$$-\;\frac{c\widehat{\mathsf{b}}}{eB}\times\left[D_1^2(\mathbf{P}_3) + \nabla\sigma_3 - \mathbf{\Pi}_2\right], \tag{6.33}$$

where the parallel component $G_{3\|}^{\mathbf{x}}$ is determined at the fourth order.

7. Fourth-order Perturbation Analysis

The fourth-order guiding-center symplectic one-form (3.14) is explicitly expressed in five parts. The first part is

$$-\,\imath_4\cdot\boldsymbol{\omega}_0 \;=\; -\,\frac{e}{c}\,\mathbf{B}\times G_4^{\mathbf{x}}\boldsymbol{\cdot}\mathsf{d}\mathbf{X}, \tag{7.1}$$

the second part is

$$-\,\imath_3\cdot\boldsymbol{\omega}_{\rm gc1} \;=\; -\,D_3\left(p_\|\,\widehat{\mathsf{b}}\right)\boldsymbol{\cdot}\mathsf{d}\mathbf{X} \;+\; G_{3\|}^{\mathbf{x}}\;\mathsf{d}p_\|, \tag{7.2}$$

the third part is

$$-\,\frac{1}{2}\,\imath_2\cdot\boldsymbol{\omega}_{\rm gc2} = \frac{1}{2}\,D_2\left(J\,\mathbf{R} - \mathbf{\Pi}_1\right)\boldsymbol{\cdot}\mathsf{d}\mathbf{X} \;-\; \frac{1}{2}\,G_2^J\;\mathsf{d}\theta \;+\; \frac{1}{2}\left(G_2^\theta \;-\; G_2^{\mathbf{x}}\boldsymbol{\cdot}\mathbf{R}^*\right)\,\mathsf{d}J, \tag{7.3}$$

where $\mathbf{R}^* \equiv \mathbf{R} - \partial\mathbf{\Pi}_1/\partial J$, the fourth part is

$$\frac{1}{4}\,\imath_2\cdot\mathsf{d}\left[\imath_1\cdot\left(\boldsymbol{\omega}_1 \;+\; \boldsymbol{\omega}_{\rm gc1}\right)\right] = \frac{1}{2}\,D_2\left[D_1(\mathbf{P}_2)\right]\boldsymbol{\cdot}\mathsf{d}\mathbf{X} \;-\; \frac{1}{2}\left(G_2^J\;\mathsf{d}\theta \;-\; G_2^\theta\;\mathsf{d}J\right)$$
$$-\;\frac{1}{2}G_2^{\mathbf{x}}\boldsymbol{\cdot}\frac{\partial D_1(\mathbf{P}_2)}{\partial u^a}\;\mathsf{d}u^a, \tag{7.4}$$

and the fifth part is

$$-\,\frac{1}{8}\,\imath_1\cdot\mathsf{d}\left[\imath_1\cdot\mathsf{d}\left(\imath_1\cdot\omega_1 \;+\; \frac{1}{3}\,\imath_1\cdot\boldsymbol{\omega}_{\rm gc1}\right)\right] = -\,\frac{1}{2}\,D_1^3(\mathbf{P}_4)\boldsymbol{\cdot}\mathsf{d}\mathbf{X} \;-\; \frac{1}{2}\,\frac{\partial D_1^2(\mathbf{P}_4)}{\partial u^a}\boldsymbol{\cdot}\boldsymbol{\rho}_0\;\mathsf{d}u^a$$
$$+\;\frac{1}{4}\left(\mathsf{d}G_1^\theta\;G_1^J \;-\; \mathsf{d}G_1^J\;G_1^\theta\right)$$
$$-\;\frac{1}{2}\left(\mathsf{G}_1\cdot\mathsf{d}F_{1a}\;\mathsf{d}u^a \;-\; \mathsf{d}F_{1a}\;G_1^a\right)$$
$$+\;\frac{1}{4}\,\mathsf{G}_1\cdot\left(\mathsf{d}G_1^J\;\mathsf{d}\theta \;-\; \mathsf{d}G_1^\theta\;\mathsf{d}J\right), \tag{7.5}$$

where

$$\mathbf{P}_4 \;\equiv\; \frac{1}{3}\,p_\|\,\widehat{\mathsf{b}} \;+\; \frac{1}{4}\,\mathbf{p}_\perp, \tag{7.6}$$

and the momentum coordinates are labeled as $u^a = (p_\|, J, \theta)$ and

$$F_{1a} \;\equiv\; \frac{\partial D_1(\mathbf{P}_4)}{\partial u^a}\boldsymbol{\cdot}\boldsymbol{\rho}_0. \tag{7.7}$$

We now combine these parts to write the components of the fourth-order guiding-center symplectic one-form (3.14) as

$$\begin{aligned}
\Gamma_{4\mathbf{x}} \equiv \boldsymbol{\Pi}_4 \;=\; & \nabla\sigma_4 \;-\; \frac{e}{c}\,\mathbf{B}\times G_4^{\mathbf{x}} \;-\; D_3\left(p_\| \,\widehat{\mathsf{b}}\right) \;+\; \frac{1}{2}\,D_2\left(J\,\mathbf{R} - \boldsymbol{\Pi}_1\right) \\
& +\frac{1}{2}\,D_2\left[D_1(\mathbf{P}_2)\right] \;-\; \frac{1}{2}\,\left[D_1^3(\mathbf{P}_4) \;-\; \nabla F_{1a}\,G_1^a\right] \;+\; \frac{1}{4}\left(G_1^J\,\nabla G_1^\theta \;-\; G_1^\theta\,\nabla G_1^J\right),
\end{aligned} \tag{7.8}$$

$$\begin{aligned}
\Gamma_{4p_\|} \equiv 0 \;=\; & \frac{\partial\sigma_4}{\partial p_\|} \;+\; G_{3\|}^{\mathbf{x}} \;-\; \frac{1}{2}\,G_2^{\mathbf{x}}\cdot\frac{\partial D_1(\mathbf{P}_2)}{\partial p_\|} \;-\; \frac{1}{2}\,\boldsymbol{\rho}_0\cdot\frac{\partial D_1^2(\mathbf{P}_4)}{\partial p_\|} \\
& -\frac{1}{2}\left(\mathsf{G}_1\cdot\mathsf{d}F_{1p_\|} \;-\; \frac{\partial F_{1a}}{\partial p_\|}\,G_1^a\right) \;+\; \frac{1}{4}\left(G_1^J\,\frac{\partial G_1^\theta}{\partial p_\|} \;-\; G_1^\theta\,\frac{\partial G_1^J}{\partial p_\|}\right),
\end{aligned} \tag{7.9}$$

$$\begin{aligned}
\Gamma_{4J} \equiv 0 \;=\; & \frac{\partial\sigma_4}{\partial J} \;+\; G_2^\theta \;-\; \frac{1}{2}\,G_2^{\mathbf{x}}\cdot\left[\mathbf{R}^* \;+\; \frac{\partial D_1(\mathbf{P}_2)}{\partial J}\right] \;-\; \frac{1}{2}\,\boldsymbol{\rho}_0\cdot\frac{\partial D_1^2(\mathbf{P}_4)}{\partial J} \\
& -\frac{1}{2}\left(\mathsf{G}_1\cdot\mathsf{d}F_{1J} \;-\; \frac{\partial F_{1a}}{\partial J}\,G_1^a\right) \;+\; \frac{1}{4}\left(G_1^J\,\frac{\partial G_1^\theta}{\partial J} \;-\; G_1^\theta\,\frac{\partial G_1^J}{\partial J} \;-\; \mathsf{G}_1\cdot\mathsf{d}G_1^\theta\right),
\end{aligned} \tag{7.10}$$

$$\begin{aligned}
\Gamma_{4\theta} \equiv 0 \;=\; & \frac{\partial\sigma_4}{\partial\theta} \;-\; G_2^J \;-\; \frac{1}{2}\,G_2^{\mathbf{x}}\cdot\frac{\partial D_1(\mathbf{P}_2)}{\partial\theta} \;-\; \frac{1}{2}\,\boldsymbol{\rho}_0\cdot\frac{\partial D_1^2(\mathbf{P}_4)}{\partial\theta} \\
& -\frac{1}{2}\left(\mathsf{G}_1\cdot\mathsf{d}F_{1\theta} \;-\; \frac{\partial F_{1a}}{\partial\theta}\,G_1^a\right) \;+\; \frac{1}{4}\left(G_1^J\,\frac{\partial G_1^\theta}{\partial\theta} \;-\; G_1^\theta\,\frac{\partial G_1^J}{\partial\theta} \;+\; \mathsf{G}_1\cdot\mathsf{d}G_1^J\right).
\end{aligned} \tag{7.11}$$

Hence, the components $G_{4\perp}^{\mathbf{x}}$ and $G_3^{p_\|}$ are obtained from Eq. (7.8), the component $G_{3\|}^{\mathbf{x}}$ is obtained from Eq. (7.9), and the components (G_2^θ, G_2^J) are obtained from Eqs. (7.10)-(7.11), respectively.

From the condition $\Gamma_{4\theta} \equiv 0$ in Eq. (7.11), we obtain the missing component $\langle G_2^J\rangle$ in Eq. (6.31):

$$\begin{aligned}
\langle G_2^J\rangle = & \frac{1}{2}\left\langle\frac{\partial G_2^{\mathbf{x}}}{\partial\theta}\cdot D_1(\mathbf{P}_2)\right\rangle \;+\; \frac{1}{4}\left\langle G_1^J\,\frac{\partial G_1^\theta}{\partial\theta} \;-\; G_1^\theta\,\frac{\partial G_1^J}{\partial\theta} \;+\; \mathsf{G}_1\cdot\mathsf{d}G_1^J\right\rangle \\
& +\frac{1}{2}\left\langle\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot D_1^2(\mathbf{P}_4)\right\rangle \;-\; \frac{1}{2}\left\langle\mathsf{G}_1\cdot\mathsf{d}F_{1\theta} \;-\; G_1^a\,\frac{\partial F_{1a}}{\partial\theta}\right\rangle.
\end{aligned} \tag{7.12}$$

After several calculations detailed in App. C, we obtain

$$\begin{aligned}
\langle G_2^J\rangle = & \frac{J^2}{2m\Omega}\left[\frac{\tau^2}{2} + \widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} - \langle\alpha_1^2\rangle - \frac{\widehat{\mathsf{b}}}{2}\cdot\nabla\times(\widehat{\mathsf{b}}\times\nabla\ln B)\right] \\
& -\frac{J}{2}\,\varrho_\|^2\left[\boldsymbol{\kappa}\cdot(3\,\boldsymbol{\kappa} - \nabla\ln B) \;+\; \nabla\cdot\boldsymbol{\kappa} - \tau^2\right].
\end{aligned} \tag{7.13}$$

When compared with Eq. (6.30), we obtain the second-order guiding-center Hamiltonian constraint

$$\begin{aligned}
\frac{p_\|}{m}\,\Pi_{2\|} \;-\; \Psi_2 = & \frac{m}{2}\,|\mathbf{v}_{\rm gc}|^2 \;-\; \boldsymbol{\Pi}_1\cdot\mathbf{v}_{\rm gc} \;+\; \frac{J}{2}\,\Omega\,\varrho_\|^2\left[2\,\langle\alpha_1^2\rangle \;-\; \boldsymbol{\kappa}\cdot(3\,\boldsymbol{\kappa} - \nabla\ln B) \;-\; \nabla\cdot\boldsymbol{\kappa}\right] \\
& +\frac{J^2}{2m}\left[\frac{1}{2}\,\tau^2 \;+\; \widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} \;-\; \langle\alpha_1^2\rangle \;-\; \frac{1}{2}\,\widehat{\mathsf{b}}\cdot\nabla\times\left(\widehat{\mathsf{b}}\times\nabla\ln B\right)\right] \\
\equiv & -\,J\,\Omega\left(\frac{J}{2\,m\Omega}\,\beta_{2\perp} \;+\; \frac{1}{2}\,\varrho_\|^2\,\beta_{2\|}\right) \;+\; \frac{p_\|^2}{2m}\,\left(\varrho_\|^2\,|\boldsymbol{\kappa}|^2\right) \;-\; \boldsymbol{\Pi}_1\cdot\mathbf{v}_{\rm gc},
\end{aligned} \tag{7.14}$$

where the second-order functions $\beta_{2\perp}$ and $\beta_{2\|}$ depend only on the guiding-center position

$$\beta_{2\perp} = -\,\frac{1}{2}\,\tau^2 \;-\; \widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} \;+\; \langle\alpha_1^2\rangle \;+\; \frac{1}{2}\,\widehat{\mathsf{b}}\cdot\nabla\times\left(\widehat{\mathsf{b}}\times\nabla\ln B\right) \;-\; \left|\widehat{\mathsf{b}}\times\nabla\ln B\right|^2 \tag{7.15}$$

$$\beta_{2\|} = -\,2\,\langle\alpha_1^2\rangle \;-\; 3\,\boldsymbol{\kappa}\cdot\left(\nabla\ln B \;-\; \boldsymbol{\kappa}\right) \;+\; \nabla\cdot\boldsymbol{\kappa}. \tag{7.16}$$

The definitions of $\langle\alpha_1^2\rangle$ and $\widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R}$ are given in App. A, and the last term in Eq. (7.14) explicitly involves the undetermined component $\mathbf{\Pi}_{1\perp}$.

We now note that, in contrast to first-order guiding-center Hamiltonian constraint (6.14), the right side of Eq. (7.14) contains terms that are constant, quadratic, and quartic in $p_\|$. Hence, since $\beta_{2\perp} \neq 0$, we cannot choose $\Psi_2 = 0$ without making $\Pi_{2\|}$ singular in $p_\|$. Hence, while a purely Hamiltonian representation of guiding-center theory is possible ($\Pi_{n\|} \equiv 0$, $n \geq 1$), a purely symplectic representation ($\Psi_n \equiv 0$, $n \geq 1$) is impossible.

8. Guiding-center Jacobian

So far we have derived the guiding-center transformation (3.1) up to second order in magnetic-field nonuniformity. We now summarize the guiding-center transformation determined by the first-order generating vector-field components

$$\begin{aligned}
G_1^{\mathbf{x}} &= -\,\boldsymbol{\rho}_0, \\
G_1^{p_\|} &= -\,p_\|\,\boldsymbol{\rho}_0\cdot\boldsymbol{\kappa} \;+\; J\,(\tau \;+\; \alpha_1)\,, \\
G_1^J &\equiv J\,\boldsymbol{\rho}_0\cdot\nabla\ln B \;-\; \varrho_\|\,G_1^{p_\|} = \boldsymbol{\rho}_0\cdot\left(J\,\nabla\ln B + \frac{p_\|^2\,\boldsymbol{\kappa}}{m\Omega}\right) - J\,\varrho_\|\,(\tau+\alpha_1), \\
G_1^\theta &= -\,\boldsymbol{\rho}_0\cdot\mathbf{R} \;+\; \varrho_\|\,\alpha_2 \;+\; \frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\left(\nabla\ln B \;+\; \frac{p_\|^2\,\boldsymbol{\kappa}}{2\,m\,J\Omega}\right),
\end{aligned}$$

and the second-order generating vector-field components

$$\begin{aligned}
G_2^{\mathbf{x}} &= \left(2\,\varrho_\|\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\boldsymbol{\kappa} \;+\; \frac{J\,\alpha_2}{m\Omega}\right)\widehat{\mathsf{b}} \;+\; \frac{1}{2}\left[\frac{p_\|^2}{m\Omega}\,(\boldsymbol{\rho}_0\cdot\boldsymbol{\kappa}) \;+\; J\,\varrho_\|\,(3\tau-\alpha_1)\right]\frac{\partial\boldsymbol{\rho}_0}{\partial J} \\
&\quad +\; \frac{1}{2}\left[\varrho_\|\,\alpha_2 \;+\; \frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\left(\nabla\ln B \;+\; \frac{p_\|^2\,\boldsymbol{\kappa}}{2m\Omega\,J}\right)\right]\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} \;-\; \mathbf{\Pi}_1\times\frac{\widehat{\mathsf{b}}}{m\Omega}, \\
G_2^{p_\|} &= p_\|\,\boldsymbol{\kappa}\cdot G_2^{\mathbf{x}} \;+\; \widehat{\mathsf{b}}\cdot\left[D_1^2(\mathbf{P}_3) + \nabla\sigma_3 - \mathbf{\Pi}_2\right], \\
G_2^J &\equiv -\,J\,G_2^{\mathbf{x}}\cdot\nabla\ln B \;-\; \varrho_\|\,G_2^{p_\|} \;-\; \Psi_2/\Omega \\
&= -\,G_2^{\mathbf{x}}\cdot\left(J\,\nabla\ln B \;+\; \frac{p_\|^2\,\boldsymbol{\kappa}}{m\,\Omega}\right) \;-\; \varrho_\|\widehat{\mathsf{b}}\cdot\left[D_1^2(\mathbf{P}_3) + \nabla\sigma_3\right] \;-\; \frac{1}{\Omega}\left(\Psi_2 \;-\; \frac{p_\|}{m}\,\Pi_{2\|}\right),
\end{aligned}$$

while $G_{3\perp}^{\mathbf{x}}$, which is given by Eq. (6.33), is not needed in this Section. The remaining components $G_{3\|}^{\mathbf{x}}$ and G_2^θ, which are determined from Eqs. (7.9)-(7.10), are not needed in what follows.

We would like to verify that the guiding-center transformation constructed so far is consistent with the guiding-center Jacobian (2.6) as expressed in terms of Lie-transform methods as Eq. (3.3). For this purpose, we will need the gyroangle-averaged components

$$\langle G_1^{p_\|}\rangle = J\,\tau, \tag{8.1}$$

$$\langle G_1^J\rangle = -\,J\,\varrho_\|\,\tau, \tag{8.2}$$

$$\langle G_2^{\mathbf{x}}\rangle = -\,\mathbf{\Pi}_1\times\frac{\widehat{\mathsf{b}}}{m\Omega} \;+\; \frac{1}{2}\left(\frac{J}{m\Omega}\,\nabla_\perp\ln B \;+\; \varrho_\|^2\,\boldsymbol{\kappa}\right), \tag{8.3}$$

$$\begin{aligned}\langle G_2^{p_\|}\rangle &= -\,\varrho_\|\widehat{\mathsf{b}}\times\boldsymbol{\kappa}\cdot\mathbf{\Pi}_1 + \varrho_\|\,\boldsymbol{\kappa}\cdot\left(J\,\nabla\ln B \;+\; \frac{p_\|^2\boldsymbol{\kappa}}{m\Omega}\right)\\ &\quad -\,\Pi_{2\|} - J\varrho_\|\left(\frac{1}{2}\,\tau^2 - \langle\alpha_1^2\rangle\right),\end{aligned} \tag{8.4}$$

$$\begin{aligned}\langle G_2^J\rangle &= \frac{J^2}{2m\Omega}\left[\frac{1}{2}\,\tau^2 \;+\; \widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} \;-\; \langle\alpha_1^2\rangle \;-\; \frac{1}{2}\,\widehat{\mathsf{b}}\cdot\nabla\times(\widehat{\mathsf{b}}\times\nabla\ln B)\right]\\ &\quad -\,\frac{1}{2}\,J\,\varrho_\|^2\left[\boldsymbol{\kappa}\cdot(3\,\boldsymbol{\kappa}-\nabla\ln B) \;+\; \nabla\cdot\boldsymbol{\kappa} \;-\; \tau^2\right],\end{aligned} \tag{8.5}$$

where Eq. (8.5) comes from from the fourth-order expression (7.13).

The guiding-center Jacobian (2.6) is given by $\mathcal{J}_{\rm gc}/\mathcal{J}_0 \equiv B_\|^{**}/B$:

$$\frac{\mathcal{J}_{\rm gc}}{\mathcal{J}_0} \;=\; 1 \;+\; \epsilon\,\varrho_\|\,\tau \;+\; \epsilon^2\left(\frac{\partial\Pi_{2\|}}{\partial p_\|} \;+\; \frac{c\,\widehat{\mathsf{b}}}{eB}\cdot\nabla\times(\mathbf{\Pi}_1 - J\,\mathbf{R})\right) \;+\; \cdots. \tag{8.6}$$

Hence, at first order, using Eqs. (6.16)-(6.17) and (6.21), we find

$$\begin{aligned}\frac{\mathcal{J}_1}{\mathcal{J}_0} &\equiv \frac{1}{B}\,\nabla\cdot\left(B\,\boldsymbol{\rho}_0\right) \;-\; \left(\frac{\partial G_1^{p_\|}}{\partial p_\|} \;+\; \frac{\partial G_1^J}{\partial J} \;+\; \frac{\partial G_1^\theta}{\partial\theta}\right)\\ &= \varrho_\|\,\tau \;\equiv\; -\left(\frac{\partial\langle G_1^{p_\|}\rangle}{\partial p_\|} \;+\; \frac{\partial\langle G_1^J\rangle}{\partial J}\right).\end{aligned} \tag{8.7}$$

In the last equality, we have used the fact that, since the guiding-center Jacobian is gyroangle-independent, we may also gyroangle-average Eq. (8.7), which greatly simplifies the calculations, since Eqs. (8.1)-(8.2) yield $\partial\langle G_1^{p_\|}\rangle/\partial p_\| = 0$ and $\partial\langle G_1^J\rangle/\partial J = -\,\varrho_\|\,\tau$.

At second order, we must verify that

$$\begin{aligned}\frac{\mathcal{J}_2}{\mathcal{J}_0} &\equiv \frac{\partial\Pi_{2\|}}{\partial p_\|} \;+\; \frac{c\,\widehat{\mathsf{b}}}{eB}\cdot\nabla\times\left(\mathbf{\Pi}_1 \;-\; J\,\mathbf{R}\right)\\ &\equiv -\,\frac{1}{B}\nabla\cdot\left(B\,\langle G_2^{\mathbf{x}}\rangle\right) \;-\; \frac{\partial}{\partial p_\|}\left(\langle G_2^{p_\|}\rangle \;+\; \frac{1}{2}\,J\,\varrho_\|\,\tau^2\right) - \frac{\partial}{\partial J}\left(\langle G_2^J\rangle \;-\; \frac{1}{2}\,J\,\varrho_\|^2\,\tau^2\right),\end{aligned} \tag{8.8}$$

where we once again used the gyroangle-averaged expressions for $(G_2^{\mathbf{x}}, G_2^{p_\|}, G_2^J)$, with $(\langle G_1^{p_\|}\rangle, \langle G_1^J\rangle) = (J\,\tau, -\,J\,\varrho_\|\tau)$. First, using Eq. (8.3), we find

$$\begin{aligned}-\,\frac{1}{B}\nabla\cdot\left(B\,\langle G_2^{\mathbf{x}}\rangle\right) &= -\,\frac{J}{2m\Omega}\,\nabla\cdot\left[\left(\widehat{\mathsf{b}}\times\nabla\ln B\right)\times\widehat{\mathsf{b}}\right] \;-\; \frac{1}{2}\,B\,\varrho_\|^2\,\nabla\cdot\left(\frac{\boldsymbol{\kappa}}{B}\right)\\ &\quad +\,\frac{c}{eB}\,\nabla\cdot\left(\mathbf{\Pi}_1\times\widehat{\mathsf{b}}\right).\end{aligned} \tag{8.9}$$

Next, using Eq. (8.4), we obtain

$$-\frac{\partial}{\partial p_{\|}}\left(\langle G_2^{p_{\|}}\rangle + \frac{1}{2}\,J\,\varrho_{\|}\,\tau^2\right) = -\frac{J}{m\Omega}\left(\langle\alpha_1^2\rangle + \frac{1}{2}\,\boldsymbol{\kappa}\cdot\nabla\ln B\right) - \frac{3}{2}\,\varrho_{\|}^2\,|\boldsymbol{\kappa}|^2 + \left(\frac{\mathbf{\Pi}_1}{m\Omega} + \varrho_{\|}\,\frac{\partial\mathbf{\Pi}_1}{\partial p_{\|}}\right)\cdot\left(\widehat{\mathsf{b}}\times\boldsymbol{\kappa}\right) + \frac{\partial\Pi_{2\|}}{\partial p_{\|}}. \tag{8.10}$$

Lastly, using Eq. (8.5), we obtain

$$-\frac{\partial}{\partial J}\left(\langle G_2^J\rangle - \frac{J}{2}\,\varrho_{\|}^2\,\tau^2\right) = -\frac{J}{m\Omega}\left[\frac{\tau^2}{2} + \widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} - \langle\alpha_1^2\rangle - \frac{\widehat{\mathsf{b}}}{2}\cdot\nabla\times\left(\widehat{\mathsf{b}}\times\nabla\ln B\right)\right] + \frac{1}{2}\,\varrho_{\|}^2\left[\boldsymbol{\kappa}\cdot(3\,\boldsymbol{\kappa} - \nabla\ln B) + \nabla\cdot\boldsymbol{\kappa}\right]. \tag{8.11}$$

By combining Eqs. (8.9)-(8.11) into Eq. (8.8), we obtain

$$\begin{aligned}\frac{\mathcal{J}_2}{\mathcal{J}_0} &= \frac{\partial\Pi_{2\|}}{\partial p_{\|}} + \frac{c\,\widehat{\mathsf{b}}}{eB}\cdot\nabla\times(\mathbf{\Pi}_1 - J\,\mathbf{R}) + \varrho_{\|}\,\frac{\partial\mathbf{\Pi}_1}{\partial p_{\|}}\cdot\left(\widehat{\mathsf{b}}\times\boldsymbol{\kappa}\right) - \frac{\tau}{m\Omega}\left(\Pi_{1\|} + \frac{1}{2}\,J\,\tau\right) \\ &\quad - \frac{J}{2m\Omega}\left\{\nabla\cdot\left[\left(\widehat{\mathsf{b}}\times\nabla\ln B\right)\times\widehat{\mathsf{b}}\right] + \boldsymbol{\kappa}\cdot\nabla\ln B - \widehat{\mathsf{b}}\cdot\nabla\times\left(\widehat{\mathsf{b}}\times\nabla\ln B\right)\right\} \\ &\quad + \frac{1}{2}\,\varrho_{\|}^2\left[\boldsymbol{\kappa}\cdot(3\,\boldsymbol{\kappa} - \nabla\ln B) + \nabla\cdot\boldsymbol{\kappa} - \nabla\cdot\boldsymbol{\kappa} - 3\,|\boldsymbol{\kappa}|^2 + \boldsymbol{\kappa}\cdot\nabla\ln B\right] \\ &= \frac{\partial\Pi_{2\|}}{\partial p_{\|}} + \frac{c\,\widehat{\mathsf{b}}}{eB}\cdot\nabla\times(\mathbf{\Pi}_1 - J\,\mathbf{R}) + \varrho_{\|}\,\frac{\partial\mathbf{\Pi}_1}{\partial p_{\|}}\cdot\left(\widehat{\mathsf{b}}\times\boldsymbol{\kappa}\right) - \frac{\tau}{m\Omega}\left(\Pi_{1\|} + \frac{1}{2}\,J\,\tau\right).\end{aligned}$$

Hence, we find

$$\frac{\mathcal{J}_2}{\mathcal{J}_0} \equiv \frac{\partial\Pi_{2\|}}{\partial p_{\|}} + \frac{c\,\widehat{\mathsf{b}}}{eB}\cdot\nabla\times(\mathbf{\Pi}_1 - J\,\mathbf{R}), \tag{8.12}$$

only if $\partial\mathbf{\Pi}_1/\partial p_{\|} \equiv 0$ and $\Pi_{1\|} \equiv -\frac{1}{2}\,J\tau$.

We see that, while the Jacobian constraints are satisfied up to second order in magnetic-field nonuniformity, we are unable to obtain a constraint on the perpendicular component $\mathbf{\Pi}_{1\perp}$. Littlejohn ((Littlejohn 1983)) chose $\mathbf{\Pi}_{1\perp} \equiv 0$ (i.e., $\mathbf{\Pi}_1 \equiv -\frac{1}{2}\,J\;\tau\,\widehat{\mathsf{b}}$) as a way to simplify the symplectic (Poisson-bracket) structure. In Sec. 10.1, we will show that $\mathbf{\Pi}_{1\perp} \equiv -\frac{1}{2}\,J\,\widehat{\mathsf{b}}\times\boldsymbol{\kappa}$ so that, with Eq. (6.15), we find that

$$\mathbf{\Pi}_1 \equiv -\frac{1}{2}\,J\,\nabla\times\widehat{\mathsf{b}}. \tag{8.13}$$

We will also show that Eq. (8.13) leads to an accurate guiding-center representation of the toroidal canonical momentum.

9. Push-forward Lagrangian Constraint

We now 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 $L(\mathbf{x},\mathbf{v};\dot{\mathbf{x}},\dot{\mathbf{v}}) = m\mathbf{v}\cdot d\mathbf{x}/dt - [m\,|\mathbf{v}|^2/2 + U(\mathbf{x})]$, we first obtain the Euler-Lagrange equation for $\mathbf{x}$: $m\,d\mathbf{v}/dt = -\nabla U$. Since the phase-space Lagrangian is independent of $d\mathbf{v}/dt$, however, we immediately obtain the Lagrangian constraint

$$\frac{\partial L}{\partial \mathbf{v}} \;=\; m\,\frac{d\mathbf{x}}{dt} \;-\; \mathbf{p} \;\equiv\; 0. \tag{9.1}$$

We would now like to obtain the guiding-center version of the Lagrangian constraint (9.1). First, using the functional definition for $d_{\rm gc}/dt$:

$$\frac{d_{\rm gc}}{dt} \;\equiv\; \mathsf{T}_{\rm gc}^{-1}\left(\frac{d}{dt}\,\mathsf{T}_{\rm gc}\right), \tag{9.2}$$

we introduce the guiding-center Lagrangian constraint

$$m\,\mathsf{T}_{\rm gc}^{-1}\left(\frac{d\mathbf{x}}{dt}\right) \;\equiv\; m\,\frac{d_{\rm gc}}{dt}\left(\mathsf{T}_{\rm gc}^{-1}\mathbf{x}\right) \;=\; m\,\left(\frac{d_{\rm gc}\mathbf{X}}{dt} + \frac{d_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{dt}\right) \;\equiv\; \mathsf{T}_{\rm gc}^{-1}\mathbf{p} \tag{9.3}$$

expressed in terms of the guiding-center velocity $d_{\rm gc}\mathbf{X}/dt$ and the guiding-center displacement velocity

$$\frac{d_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{dt} \;=\; \epsilon^{-1}\,\frac{\partial\Psi}{\partial J}\,\frac{\partial\boldsymbol{\rho}_{\rm gc}}{\partial\theta} \;+\; \frac{d_{\rm gc}\mathbf{X}}{dt}\boldsymbol{\cdot}\nabla^{*}\boldsymbol{\rho}_{\rm gc} \;+\; \frac{d_{\rm gc}p_{\|}}{dt}\,\frac{\partial\boldsymbol{\rho}_{\rm gc}}{\partial p_{\|}}, \tag{9.4}$$

(which includes the polarization velocity $d\langle\boldsymbol{\rho}_{\rm gc}\rangle/dt$). Here, the guiding-center displacement is expanded as

$$\boldsymbol{\rho}_{\rm gc} \;\equiv\; \mathsf{T}_{\rm gc}^{-1}\mathbf{x} \;-\; \mathbf{X} \;=\; \epsilon\,\boldsymbol{\rho}_0 \;+\; \epsilon^2\,\boldsymbol{\rho}_1 \;+\; \epsilon^3\,\boldsymbol{\rho}_2 + \cdots, \tag{9.5}$$

where the higher-order gyroradius corrections are

$$\boldsymbol{\rho}_1 = -\,G_2^{\mathbf{x}} \;-\; \frac{1}{2}\,\mathsf{G}_1\cdot\mathsf{d}\boldsymbol{\rho}_0, \tag{9.6}$$

$$\boldsymbol{\rho}_2 = -\,G_3^{\mathbf{x}} - \mathsf{G}_2\cdot\mathsf{d}\boldsymbol{\rho}_0 + \frac{1}{6}\,\mathsf{G}_1\cdot\mathsf{d}(\mathsf{G}_1\cdot\mathsf{d}\boldsymbol{\rho}_0). \tag{9.7}$$

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 $n \geq 1$.

In Eq. (9.3), the push-forward of the particle momentum $\mathsf{T}_{\rm gc}^{-1}\mathbf{p}$ can be expanded up to second order in ϵ as

$$\begin{aligned}
\mathsf{T}_{\rm gc}^{-1}\mathbf{p} = \mathbf{p} \;+\; \epsilon\,&\left[\boldsymbol{\rho}_0\boldsymbol{\cdot}\nabla\mathbf{p} \;-\; \left(G_1^{p_\|}\,\widehat{\mathsf{b}} \;+\; G_1^{J}\,\frac{\partial\mathbf{p}_\perp}{\partial J} \;+\; G_1^{\theta}\,\frac{\partial\mathbf{p}_\perp}{\partial\theta}\right)\right] \\
&-\,\epsilon^2\left[G_2^{\mathbf{x}}\boldsymbol{\cdot}\nabla\mathbf{p} \;+\; \left(G_2^{p_\|}\,\widehat{\mathsf{b}} \;+\; G_2^{J}\,\frac{\partial\mathbf{p}_\perp}{\partial J} \;+\; G_2^{\theta}\,\frac{\partial\mathbf{p}_\perp}{\partial\theta}\right)\right] \\
&+\,\frac{\epsilon^2}{2}\,\mathsf{G}_1\cdot\mathsf{d}\left(G_1^{p_\|}\,\widehat{\mathsf{b}} \;+\; G_1^{J}\,\frac{\partial\mathbf{p}_\perp}{\partial J} \;+\; G_1^{\theta}\,\frac{\partial\mathbf{p}_\perp}{\partial\theta} \;-\; \boldsymbol{\rho}_0\boldsymbol{\cdot}\nabla\mathbf{p}\right) \;+\; \cdots,
\end{aligned} \tag{9.8}$$

while the push-forward of the particle velocity is expanded up to second order in ϵ as

$$\begin{aligned}
\frac{d_{\rm gc}\mathbf{X}}{dt} \;+\; \frac{d_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{dt} = &\left(\frac{d_0\mathbf{X}}{dt} \;+\; \Omega\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right) \;+\; \epsilon\,\left(\frac{d_1\mathbf{X}}{dt} \;+\; \Omega\,\frac{\partial\boldsymbol{\rho}_1}{\partial\theta} \;+\; \frac{d_0\mathbf{X}}{dt}\boldsymbol{\cdot}\nabla_0^{*}\boldsymbol{\rho}_0\right) \\
&+\,\epsilon^2\,\left[\frac{d_2\mathbf{X}}{dt} \;+\; \Omega\,\frac{\partial\boldsymbol{\rho}_2}{\partial\theta} \;+\; \frac{\partial}{\partial J}\left(\Psi_2 - \frac{p_\|}{m}\,\Pi_{2\|}\right)\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right. \\
&\left.+\;\frac{d_1\mathbf{X}}{dt}\boldsymbol{\cdot}\nabla_0^{*}\boldsymbol{\rho}_0 \;+\; \frac{d_0\mathbf{X}}{dt}\boldsymbol{\cdot}\nabla_0^{*}\boldsymbol{\rho}_1 \;+\; \frac{d_0p_\|}{dt}\,\frac{\partial\boldsymbol{\rho}_1}{\partial p_\|}\right] + \cdots,
\end{aligned} \tag{9.9}$$

where we used $m\,d_0\mathbf{X}/dt = p_\|\,\widehat{\mathsf{b}}$, $\nabla_0^{*} \equiv \nabla + (\mathbf{R} - \partial\boldsymbol{\Pi}_1/\partial J)\,\partial/\partial\theta$, and $\partial\boldsymbol{\rho}_0/\partial p_\| \equiv 0$ with

$\Psi_1 \equiv 0$. At the lowest order in ϵ, the guiding-center Lagrangian constraint (9.3) yields

$$\mathbf{p} \;\equiv\; p_\parallel\,\widehat{\mathsf{b}} \;+\; m\,\Omega\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}. \tag{9.10}$$

At the next orders, we used the expansions $d_{\rm gc}Z^\alpha/dt \equiv \sum_n^\infty \epsilon^n\; d_nZ^\alpha/dt$ (which now includes the expansion of $B_\parallel^{**}$) to obtain

$$\begin{aligned} m\,\frac{d_1\mathbf{X}}{dt} &= \frac{1}{\Omega}\left(\frac{p_\parallel^2}{m}\,\nabla\times\widehat{\mathsf{b}} + J\,\widehat{\mathsf{b}}\times\nabla\Omega\right) \;-\; p_\parallel\;\left(\varrho_\parallel\,\tau\right)\,\widehat{\mathsf{b}} \\ &= \widehat{\mathsf{b}}\times\left(J\,\nabla\ln B \;+\; \frac{p_\parallel^2}{m\Omega}\,\boldsymbol{\kappa}\right) \;\equiv\; m\,\mathbf{v}_{\rm gc}, \end{aligned} \tag{9.11}$$

$$\begin{aligned} m\,\frac{d_2\mathbf{X}}{dt} &= m\,\left(\frac{\partial\Psi_2}{\partial p_\parallel} - \frac{p_\parallel}{m}\,\frac{\partial\Pi_{2\parallel}}{\partial p_\parallel}\right)\widehat{\mathsf{b}} - m\,(\varrho_\parallel\tau)\,\mathbf{v}_{\rm gc} \\ &\quad + \varrho_\parallel\,\left[\nabla\times\left(\mathbf{\Pi}_1 \;-\; J\,\mathbf{R}\right) - \widehat{\mathsf{b}}\,\widehat{\mathsf{b}}\boldsymbol{\cdot}\nabla\times\left(\mathbf{\Pi}_1 \;-\; J\,\mathbf{R}\right)\right], \end{aligned} \tag{9.12}$$

where we used $\partial\mathbf{\Pi}_1/\partial p_\parallel \equiv 0$.

9.1. *First-order constraint*

At first order, the guiding-center Lagrangian constraint (9.3) yields

$$-\,\mathsf{G}_1\cdot\mathsf{d}\mathbf{p} = m\,\left(\mathbf{v}_{\rm gc} \;+\; \Omega\,\frac{\partial\boldsymbol{\rho}_1}{\partial\theta} \;+\; \frac{d_0\boldsymbol{\rho}_0}{dt}\right), \tag{9.13}$$

where

$$\frac{d_0\boldsymbol{\rho}_0}{dt} = \frac{p_\parallel}{m}\left[-\,(\boldsymbol{\rho}_0\boldsymbol{\cdot}\boldsymbol{\kappa})\,\widehat{\mathsf{b}} \;+\; \frac{1}{2}\,\tau\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} \;+\; \frac{1}{2}\left(\nabla\boldsymbol{\cdot}\widehat{\mathsf{b}}\right)\,\boldsymbol{\rho}_0\right], \tag{9.14}$$

$$\begin{aligned} \Omega\frac{\partial\boldsymbol{\rho}_1}{\partial\theta} &\equiv \frac{p_\parallel}{m}\left[2\,(\boldsymbol{\rho}_0\boldsymbol{\cdot}\boldsymbol{\kappa})\widehat{\mathsf{b}} \;-\; \frac{1}{2}\,(\tau+\alpha_1)\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} \;-\; \alpha_2\,\boldsymbol{\rho}_0\right] \\ &\quad + \frac{J}{m}\left(\alpha_1\,\widehat{\mathsf{b}} \;-\; 2\,\mathsf{a}_1\boldsymbol{\cdot}\nabla\ln B\right). \end{aligned} \tag{9.15}$$

The first-order guiding-center Lagrangian constraint (9.13) yields the following component equations

$$(\boldsymbol{\rho}_0\boldsymbol{\cdot}\nabla\mathbf{p})\boldsymbol{\cdot}\widehat{\mathsf{b}} \;-\; G_1^{p_\parallel} = m\widehat{\mathsf{b}}\boldsymbol{\cdot}\left(\mathbf{v}_{\rm gc} \;+\; \Omega\,\frac{\partial\boldsymbol{\rho}_1}{\partial\theta} \;+\; \frac{d_0\boldsymbol{\rho}_0}{dt}\right), \tag{9.16}$$

$$(\boldsymbol{\rho}_0\boldsymbol{\cdot}\nabla\mathbf{p})\boldsymbol{\cdot}\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} \;-\; G_1^J = m\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\boldsymbol{\cdot}\left(\mathbf{v}_{\rm gc} \;+\; \Omega\,\frac{\partial\boldsymbol{\rho}_1}{\partial\theta} \;+\; \frac{d_0\boldsymbol{\rho}_0}{dt}\right), \tag{9.17}$$

$$(\boldsymbol{\rho}_0\boldsymbol{\cdot}\nabla\mathbf{p})\boldsymbol{\cdot}\frac{\partial\boldsymbol{\rho}_0}{\partial J} \;+\; G_1^\theta = m\frac{\partial\boldsymbol{\rho}_0}{\partial J}\boldsymbol{\cdot}\left(\mathbf{v}_{\rm gc} \;+\; \Omega\,\frac{\partial\boldsymbol{\rho}_1}{\partial\theta} \;+\; \frac{d_0\boldsymbol{\rho}_0}{dt}\right), \tag{9.18}$$

The parallel equation (9.16) becomes

$$J\,\left(\tau \;+\; 2\,\alpha_1\right) \;-\; G_1^{p_\parallel} \;=\; m\Omega\,\frac{\partial\boldsymbol{\rho}_1}{\partial\theta}\boldsymbol{\cdot}\widehat{\mathsf{b}} \;-\; p_\parallel\;\boldsymbol{\rho}_0\boldsymbol{\cdot}\boldsymbol{\kappa},$$

which yields the same expression (6.16) for $G_1^{p_\parallel}$:

$$G_1^{p_\parallel} \;=\; -\,p_\parallel\;\boldsymbol{\rho}_0\boldsymbol{\cdot}\boldsymbol{\kappa} \;+\; J\,\left(\tau \;+\; \alpha_1\right). \tag{9.19}$$

The remaining equations (9.17)-(9.18) yield the components G_1^J and G_1^θ.

9.2. *Second-order constraint*

At second order, the guiding-center Lagrangian constraint (9.3) yields

$$
\begin{aligned}
&-\,G_2^{\mathbf{x}}\cdot\nabla\mathbf{p}\;-\;\left(G_2^{p_\|}\,\widehat{\mathsf{b}}\;+\;G_2^J\,\frac{\partial\mathbf{p}_\perp}{\partial J}\;+\;G_2^\theta\,\frac{\partial\mathbf{p}_\perp}{\partial\theta}\right)+\frac{1}{2}\,\mathsf{G}_1\cdot\mathsf{d}\,(\mathsf{G}_1\cdot\mathsf{d}\mathbf{p}) \qquad (9.20)\\
&=\;m\,\frac{d_2\mathbf{X}}{dt}+m\Omega\,\frac{\partial\boldsymbol{\rho}_2}{\partial\theta}+\frac{\partial}{\partial J}\left(\Psi_2-\frac{p_\|}{m}\,\Pi_{2\|}\right)\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}+m\,\frac{d_1\mathbf{X}}{dt}\cdot\nabla_0^*\boldsymbol{\rho}_0+m\,\frac{d_0\boldsymbol{\rho}_1}{dt}.
\end{aligned}
$$

The parallel component of the gyroangle-averaged second-order constraint equation (9.20) yields

$$
\begin{aligned}
m\left(\frac{p_\|}{m}\,\frac{\partial\Pi_{2\|}}{\partial p_\|}\;-\;\frac{\partial\Psi_2}{\partial p_\|}\right)&=\langle G_2^{p_\|}\rangle\;+\;m\,\frac{d_0\langle\boldsymbol{\rho}_1\rangle}{dt}\cdot\widehat{\mathsf{b}}\;-\;\left\langle G_2^{\mathbf{x}}\cdot\nabla\widehat{\mathsf{b}}\cdot\mathbf{p}_\perp\right\rangle\\
&\quad-\,\frac{1}{2}\left\langle\mathsf{G}_1\cdot\,\mathsf{d}\,(\mathsf{G}_1\cdot\mathsf{d}\mathbf{p})\right\rangle\cdot\widehat{\mathsf{b}}. \qquad (9.21)
\end{aligned}
$$

If we combine this equation with Eq. (6.27):

$$
\Pi_{2\|}\;=\;-\,\langle G_2^{p_\|}\rangle\;+\;p_\|\,\boldsymbol{\kappa}\cdot\langle G_2^{\mathbf{x}}\rangle\;+\;\widehat{\mathsf{b}}\cdot\,\langle D_1^2(\mathbf{P}_3)\rangle, \qquad (9.22)
$$

the contributions from $\langle G_2^{p_\|}\rangle$ cancel out when Eqs. (9.21)-(9.22) are combined and we obtain the second-order equation

$$
\begin{aligned}
m\,\frac{\partial}{\partial p_\|}\left(\frac{p_\|}{m}\,\Pi_{2\|}\;-\;\Psi_2\right)&=m\,\frac{d_0\langle\boldsymbol{\rho}_1\rangle}{dt}\cdot\widehat{\mathsf{b}}\;+\;p_\|\,\boldsymbol{\kappa}\cdot\langle G_2^{\mathbf{x}}\rangle\;-\;\left\langle G_2^{\mathbf{x}}\cdot\nabla\widehat{\mathsf{b}}\cdot\mathbf{p}_\perp\right\rangle\\
&\quad+\,\widehat{\mathsf{b}}\cdot\,\langle D_1^2(\mathbf{P}_3)\rangle\;-\;\frac{1}{2}\left\langle\mathsf{G}_1\cdot\,\mathsf{d}\,(\mathsf{G}_1\cdot\mathsf{d}\mathbf{p})\right\rangle\cdot\widehat{\mathsf{b}}. \qquad (9.23)
\end{aligned}
$$

In App. D, the right side is explicitly calculated as

$$
m\,\frac{\partial}{\partial p_\|}\left(\frac{p_\|}{m}\,\Pi_{2\|}\;-\;\Psi_2\right)\;=\;2\,p_\|\,\varrho_\|^2\,|\boldsymbol{\kappa}|^2\;-\;2\,\varrho_\|\,\widehat{\mathsf{b}}\times\boldsymbol{\kappa}\cdot\mathbf{\Pi}_1\;-\;J\,\varrho_\|\,\beta_{2\|}, \qquad (9.24)
$$

which can clearly be recovered from the second-order guiding-center Hamiltonian constraint (7.14).

10. Guiding-center Polarization and Toroidal Canonical Momentum

So far we have been unable to find a way to determine the perpendicular component $\mathbf{\Pi}_{1\perp}$ within guiding-center Lie-transform perturbation theory. The guiding-center Jacobian constraint tells us that $\partial\mathbf{\Pi}_1/\partial p_\| \equiv 0$ and $\Pi_{1\|} = -\,\frac{1}{2}\,J\,\widehat{\mathsf{b}}\cdot\nabla\times\widehat{\mathsf{b}} \equiv -\,\frac{1}{2}\,J\,\tau$.

10.1. *Guiding-center Polarization*

We show how $\mathbf{\Pi}_{1\perp}$ can be determined by requiring that the guiding-center transformation yields the guiding-center polarization obtained by Pfirsch (Pfirsch 1984) and Kaufman (Kaufman 1986).

The guiding-center displacement $\boldsymbol{\rho}_{\rm gc} \equiv \mathsf{T}_{\rm gc}^{-1}\mathbf{x} - \mathbf{X}$ is explicitly expressed as

$$
\boldsymbol{\rho}_{\rm gc}\;=\;-\,\epsilon\,G_1^{\mathbf{x}}\;-\;\epsilon^2\,G_2^{\mathbf{x}}\;+\;\frac{\epsilon^2}{2}\,\mathsf{G}_1\cdot\mathsf{d}G_1^{\mathbf{x}}\;+\;\cdots\;\equiv\;\epsilon\,\boldsymbol{\rho}_0\;+\;\epsilon^2\,\boldsymbol{\rho}_1\;+\;\cdots, \qquad (10.1)
$$

where the first-order guiding-center displacement is

$$
\begin{aligned}
\boldsymbol{\rho}_1 &= -\,G_2^{\mathbf{x}} \;+\; \frac{1}{2}\,\boldsymbol{\rho}_0\cdot\nabla\boldsymbol{\rho}_0 \;-\; \frac{1}{2}\left(G_1^J\,\frac{\partial\boldsymbol{\rho}_0}{\partial J} \;+\; G_1^\theta\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right) \\
&= -\left(G_{2\|}^{\mathbf{x}} \;+\; \frac{1}{2}\,\boldsymbol{\rho}_0\cdot\nabla\widehat{\mathsf{b}}\cdot\boldsymbol{\rho}_0\right)\widehat{\mathsf{b}} \;-\; \varrho_\|\tau\,\boldsymbol{\rho}_0 \;+\; \boldsymbol{\Pi}_1\times\frac{\widehat{\mathsf{b}}}{m\Omega} \\
&\quad -\;\left[G_1^J\,\frac{\partial\boldsymbol{\rho}_0}{\partial J} \;+\; \left(G_1^\theta \;+\; \boldsymbol{\rho}_0\cdot\mathbf{R}\right)\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right].
\end{aligned} \tag{10.2}
$$

Next, we compute the gyroangle-average $\langle\boldsymbol{\rho}_1\rangle$ and obtain

$$
\begin{aligned}
\langle\boldsymbol{\rho}_1\rangle &= -\,\frac{J}{m\Omega}\left[\frac{1}{2}\,(\nabla\cdot\widehat{\mathsf{b}})\,\widehat{\mathsf{b}} \;+\; \frac{3}{2}\,\nabla_\perp\ln B\right] \;-\; \varrho_\|^2\,\boldsymbol{\kappa} \;+\; \boldsymbol{\Pi}_1\times\frac{\widehat{\mathsf{b}}}{m\Omega} \\
&\equiv -\,\frac{1}{m\Omega}\left(J\,\nabla_\perp\ln B \;+\; \frac{p_\|^2\,\boldsymbol{\kappa}}{m\,\Omega}\right) \;+\; \nabla\cdot\left[\frac{J}{2\,m\Omega}\left(\mathbf{I} \;-\; \widehat{\mathsf{b}}\widehat{\mathsf{b}}\right)\right] \\
&\quad +\;\left(\frac{J}{2}\,\widehat{\mathsf{b}}\times\boldsymbol{\kappa} \;+\; \boldsymbol{\Pi}_1\right)\times\frac{\widehat{\mathsf{b}}}{m\Omega}.
\end{aligned} \tag{10.3}
$$

Lastly, the guiding-center polarization density is defined as the first-order expression

$$
\begin{aligned}
\boldsymbol{\pi}_{\rm gc}^{(1)} &\equiv e\,\langle\boldsymbol{\rho}_1\rangle \;-\; e\,\nabla\cdot\left(\left\langle\frac{\boldsymbol{\rho}_0\boldsymbol{\rho}_0}{2}\right\rangle\right) \;=\; -\,\frac{e}{m\Omega}\left(J\,\nabla_\perp\ln B \;+\; \frac{p_\|^2\,\boldsymbol{\kappa}}{m\,\Omega}\right) \\
&\quad +\;\left(\frac{J}{2}\,\widehat{\mathsf{b}}\times\boldsymbol{\kappa} \;+\; \boldsymbol{\Pi}_1\right)\times\frac{\widehat{\mathsf{b}}}{m\Omega},
\end{aligned} \tag{10.4}
$$

which yields the Pfirsch-Kaufman formula

$$
\boldsymbol{\pi}_{\rm gc}^{(1)} \;\equiv\; e\,\widehat{\mathsf{b}}\times\frac{\mathbf{v}_{\rm gc}}{\Omega}, \tag{10.5}
$$

only if we use the definition

$$
\boldsymbol{\Pi}_{1\perp} \;\equiv\; -\,\frac{J}{2}\,\widehat{\mathsf{b}}\times\boldsymbol{\kappa}. \tag{10.6}
$$

Hence, by combining with the condition (6.15), $\Pi_{1\|} \equiv \widehat{\mathsf{b}}\cdot\boldsymbol{\Pi}_1 = -\,\frac{1}{2}\,J\,\tau$, we find

$$
\boldsymbol{\Pi}_1 \;=\; -\,\frac{J}{2}\left(\tau\,\widehat{\mathsf{b}} \;+\; \widehat{\mathsf{b}}\times\boldsymbol{\kappa}\right) \;=\; -\,\frac{J}{2}\,\nabla\times\widehat{\mathsf{b}}, \tag{10.7}
$$

and

$$
\boldsymbol{\rho}_1 \;\equiv\; \widehat{\mathsf{b}}\times\frac{\mathbf{v}_{\rm gc}}{\Omega} \;+\; \nabla\cdot\left[\frac{J}{2\,m\Omega}\left(\mathbf{I} - \widehat{\mathsf{b}}\,\widehat{\mathsf{b}}\right)\right] \;+\; \widetilde{\boldsymbol{\rho}}_1, \tag{10.8}
$$

with the gyroangle-dependent part $\widetilde{\boldsymbol{\rho}}_1 \equiv \boldsymbol{\rho}_1 - \langle\boldsymbol{\rho}_1\rangle$ is

$$
\begin{aligned}
\widetilde{\boldsymbol{\rho}}_1 &= -\,\varrho_\|\left[2\left(\boldsymbol{\kappa}\cdot\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right)\widehat{\mathsf{b}} \;+\; \frac{1}{2}\,(\tau - \alpha_1)\,\boldsymbol{\rho}_0 \;+\; \alpha_2\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right] \\
&\quad +\;\frac{J}{m\Omega}\left(\alpha_2\widehat{\mathsf{b}} \;-\; 2\,\mathsf{a}_2\cdot\nabla\ln B\right).
\end{aligned} \tag{10.9}
$$

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

$$
\Gamma_{\rm gc} \;=\; \left(\frac{e}{\epsilon\,c}\,\mathbf{A} \;+\; p_\|\,\widehat{\mathsf{b}} \;-\; \frac{\epsilon}{2}\,J\,\nabla\times\widehat{\mathsf{b}}\right)\cdot\mathsf{d}\mathbf{X} \;+\; \epsilon\,J\,\left(\mathsf{d}\theta \;-\; \mathbf{R}\cdot\mathsf{d}\mathbf{X}\right), \tag{10.10}
$$

when terms up to first order in magnetic-field nonuniformity are retained. In Eq. (10.10), we have retained the guiding-center polarization contribution to $\mathbf{\Pi}_1 \equiv -\frac{1}{2}\,J\,\nabla\times\widehat{\mathsf{b}}$. We now show that this polarization correction enables us obtain an exact expression for the guiding-center toroidal canonical momentum up to second order in ϵ (i.e., first order in magnetic-field nonuniformity).

10.2. *Guiding-center Toroidal Canonical Momentum*

There is now well-established connection between polarization and the conservation of toroidal canonical momentum in an axisymmetric magnetic field, here represented as

$$\mathbf{B} \;=\; B_\varphi(\psi)\,\nabla\varphi \;+\; \nabla\varphi\times\nabla\psi, \tag{10.11}$$

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. (10.11), 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 (10.10):

$$\begin{aligned} P_{\mathrm{gc}\varphi} &\equiv \left[\frac{e}{\epsilon\,c}\,\mathbf{A} \;+\; p_\|\,\widehat{\mathsf{b}} \;-\; \epsilon\,J\left(\mathbf{R} \;+\; \frac{1}{2}\nabla\times\widehat{\mathsf{b}}\right)\right]\cdot\frac{\partial\mathbf{X}}{\partial\varphi} \\ &= -\,\frac{e}{\epsilon\,c}\,\psi \;+\; p_\|\,b_\varphi \;-\; \epsilon\,J\left[b_{\mathsf{z}} \;+\; \nabla\cdot\left(\widehat{\mathsf{b}}\times\frac{1}{2}\mathcal{R}^2\,\nabla\varphi\right) \;+\; \widehat{\mathsf{b}}\cdot\nabla\times\left(\frac{1}{2}\mathcal{R}^2\,\nabla\varphi\right)\right], \end{aligned} \tag{10.12}$$

where we used $\mathbf{R}\cdot\partial\mathbf{X}/\partial\varphi\equiv b_{\mathsf{z}}$ (i.e., the component of $\widehat{\mathsf{b}}$ along the symmetry axis $\widehat{\mathsf{z}}$ 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 any two vector fields $\mathbf{F}$ and $\mathbf{G}$. Next, we use

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

and

$$\widehat{\mathsf{b}}\times\frac{1}{2}\mathcal{R}^2\,\nabla\varphi \;=\; \frac{1}{2B}\left(B_\varphi\,\nabla\varphi+\nabla\varphi\times\nabla\psi\right)\times\frac{\partial\mathbf{X}}{\partial\varphi} \;=\; \frac{1}{2B}\,\nabla\psi,$$

so that Eq. (10.12) becomes

$$P_{\mathrm{gc}\varphi} \;=\; -\,\frac{e}{\epsilon\,c}\,\psi \;+\; p_\|\,b_\varphi \;-\; \epsilon\left[2\,J\,b_{\mathsf{z}} \;+\; \nabla\cdot\left(\frac{J}{2\,m\Omega}\,\frac{e}{c}\,\nabla\psi\right)\right]. \tag{10.13}$$

Here, we suspect that the last term in Eq. (10.13) is related to the second-order finite-Larmor-radius (FLR) correction to the first term.

To prove this relation, we introduce the guiding-center magnetic flux

$$\begin{aligned} \psi_{\mathrm{gc}} \equiv \left\langle\mathsf{T}_{\mathrm{gc}}^{-1}\psi\right\rangle &= \left\langle\psi+\epsilon\boldsymbol{\rho}_0\cdot\nabla\psi-\epsilon^2\left[G_2^{\mathbf{x}}\cdot\nabla\psi+\frac{1}{2}\,\mathsf{G}_1\cdot\mathsf{d}\left(\boldsymbol{\rho}_0\cdot\nabla\psi\right)\right]+\cdots\right\rangle \\ &= \psi \;+\; \epsilon^2\left(\langle\boldsymbol{\rho}_1\rangle\cdot\nabla\psi \;+\; \frac{1}{2}\,\langle\boldsymbol{\rho}_0\boldsymbol{\rho}_0\rangle : \nabla\nabla\psi\right)+\cdots, \end{aligned} \tag{10.14}$$

where we used the definition $\boldsymbol{\rho}_1\equiv -\,G_2^{\mathbf{x}}-\frac{1}{2}\,\mathsf{G}_1\cdot\mathsf{d}\boldsymbol{\rho}_0$. Next, using Eq. (10.8), we obtain

$$\begin{aligned} \psi_{\mathrm{gc}} &= \psi+\epsilon^2\left\{\widehat{\mathsf{b}}\times\frac{\mathbf{v}_{\mathrm{gc}}}{\Omega}\cdot\nabla\psi+\nabla\cdot\left[\frac{J}{2\,m\Omega}(\mathbf{I}-\widehat{\mathsf{b}}\widehat{\mathsf{b}})\right]\cdot\nabla\psi+\frac{J}{2\,m\Omega}(\mathbf{I}-\widehat{\mathsf{b}}\widehat{\mathsf{b}}) : \nabla\nabla\psi\right\} \\ &= \psi \;+\; \epsilon^2\left[\nabla\cdot\left(\frac{J}{2\,m\Omega}\,\nabla\psi\right) \;+\; \widehat{\mathsf{b}}\times\frac{\mathbf{v}_{\mathrm{gc}}}{\Omega}\cdot\nabla\psi\right]. \end{aligned} \tag{10.15}$$

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

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

Hence, the final expression for the guiding-center toroidal canonical momentum defined by Eq. (10.13) is

$$P_{{\rm gc}\varphi} \;=\; -\,\frac{e}{\epsilon\,c}\,\psi_{\rm gc} \;+\; m\left(\frac{d_0\mathbf{X}}{dt} \;+\;\epsilon\,\frac{d_1\mathbf{X}}{dt}\right)\cdot\frac{\partial\mathbf{X}}{\partial\varphi} \;-\; 2\,\epsilon\,J\,b_{\mathsf{z}}, \tag{10.16}$$

where $d_0\mathbf{X}/dt \equiv (p_\|/m)\,\widehat{\mathsf{b}}$ 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. (10.16) might be puzzling until we consider the guiding-center transformation of the particle toroidal canonical momentum

$$\begin{aligned}
P_{{\rm gc}\varphi} \equiv \left\langle \mathsf{T}_{\rm gc}^{-1}\,P_\varphi\right\rangle \;&=\; \left\langle \mathsf{T}_{\rm gc}^{-1}\left(-\,\frac{e}{\epsilon\,c}\,\psi \;+\; m\,\mathbf{v}\cdot\frac{\partial\mathbf{x}}{\partial\varphi}\right)\right\rangle \\
&= -\,\frac{e}{\epsilon\,c}\,\langle\mathsf{T}_{\rm gc}^{-1}\psi\rangle \;+\; m\,\left\langle\left(\mathsf{T}_{\rm gc}^{-1}\frac{d\mathbf{x}}{dt}\right)\cdot\left(\mathsf{T}_{\rm gc}^{-1}\frac{\partial\mathbf{x}}{\partial\varphi}\right)\right\rangle \\
&= -\,\frac{e}{\epsilon\,c}\,\psi_{\rm gc} \;+\; m\,\left\langle\left(\frac{d_{\rm gc}\mathbf{X}}{dt} + \frac{d_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{dt}\right)\cdot\left(\frac{\partial_{\rm gc}\mathbf{X}}{\partial\varphi} + \frac{\partial_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{\partial\varphi}\right)\right\rangle \\
&= -\,\frac{e}{\epsilon\,c}\,\psi_{\rm gc} \;+\; m\left(\frac{d_0\mathbf{X}}{dt} \;+\;\epsilon\,\frac{d_1\mathbf{X}}{dt}\right)\cdot\frac{\partial\mathbf{X}}{\partial\varphi} \;+\;\epsilon\,m\Omega\left\langle\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\frac{\partial\boldsymbol{\rho}_0}{\partial\varphi}\right\rangle + \cdots.
\end{aligned} \tag{10.17}$$

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

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

and we recover the guiding-center toroidal canonical momentum (10.16) from the guiding-center transformation of the particle toroidal canonical momentum (10.17).

Lastly, we note that the guiding-center toroidal canonical momentum $P_{{\rm gc}\varphi}$ is defined as the guiding-center push-forward of the particle toroidal canonical momentum P_φ:

$$P_{{\rm gc}\varphi} \;=\; \mathsf{T}_{\rm gc}^{-1}P_\varphi \;=\; -\,\frac{e}{\epsilon c}\,\mathsf{T}_{\rm gc}^{-1}\psi \;+\; m\left(\frac{d_{\rm gc}\mathbf{X}}{dt} \;+\; \frac{d_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{dt}\right)\cdot\left(\frac{\partial_{\rm gc}\mathbf{X}}{\partial\varphi} \;+\; \frac{\partial_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{\partial\varphi}\right), \tag{10.18}$$

which guarantees the invariance of the guiding-center toroidal canonical momentum $P_{{\rm gc}\varphi}$:

$$\frac{d_{\rm gc}P_{{\rm gc}\varphi}}{dt} \;\equiv\; \mathsf{T}_{\rm gc}^{-1}\left(\frac{dP_\varphi}{dt}\right) \;=\; 0. \tag{10.19}$$

We have shown in Eq. (10.17), however, that $P_{{\rm gc}\varphi} \equiv \langle\mathsf{T}_{\rm gc}^{-1}P_\varphi\rangle$, since $P_{{\rm gc}\varphi}$ is defined as the toroidal component of the gyroangle-independent guiding-center symplectic Lagrange one-form (10.10). Hence, the gyroangle-dependent terms in $\mathsf{T}_{\rm gc}^{-1}P_\varphi - \langle\mathsf{T}_{\rm gc}^{-1}P_\varphi\rangle$ must vanish identically, which is proved up to second order in ϵ (first order in ϵ_B) in App. G.

11. Summary

A systematic derivation of the higher-order 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 (10.10) is

$$\left\{F,\, G\right\}_{\rm gc} = \epsilon^{-1}\left(\frac{\partial F}{\partial\theta}\frac{\partial G}{\partial J} \;-\; \frac{\partial F}{\partial J}\frac{\partial G}{\partial\theta}\right) \;+\; \frac{\mathbf{B}^{*}}{B_{\|}^{*}}\boldsymbol{\cdot}\left(\nabla^{*}F\,\frac{\partial G}{\partial p_{\|}} \;-\; \frac{\partial F}{\partial p_{\|}}\,\nabla^{*}G\right) \\ -\; \frac{\epsilon\, c\widehat{\mathsf{b}}}{e\,B_{\|}^{*}}\boldsymbol{\cdot}\nabla^{*}F\times\nabla^{*}G, \tag{11.1}$$

where $\nabla^{*}\equiv\nabla+(\mathbf{R}+\frac{1}{2}\,\nabla\times\widehat{\mathsf{b}})\,\partial/\partial\theta$ and

$$\mathbf{B}^{*}\equiv\nabla\times\left[\mathbf{A} \;+\; \epsilon\,\frac{c\,p_{\|}}{e}\,\widehat{\mathsf{b}} \;-\; \epsilon^{2}\,\frac{cJ}{e}\,\left(\mathbf{R} \;+\; \frac{1}{2}\,\nabla\times\widehat{\mathsf{b}}\right)\right], \tag{11.2}$$

$$B_{\|}^{*}\equiv\widehat{\mathsf{b}}\boldsymbol{\cdot}\mathbf{B}^{*} \;=\; B\left[1 \;+\; \epsilon\,\varrho_{\|}\,\tau \;-\; \epsilon^{2}\,\frac{J}{m\Omega}\,\widehat{\mathsf{b}}\boldsymbol{\cdot}\nabla\times\left(\mathbf{R} \;+\; \frac{1}{2}\,\nabla\times\widehat{\mathsf{b}}\right)\right], \tag{11.3}$$

$$\mathbf{R}^{*}\equiv\mathbf{R} \;-\; \epsilon^{-1}\,\frac{\partial\mathbf{\Pi}}{\partial J} \;=\; \mathbf{R} \;+\; \frac{1}{2}\,\nabla\times\widehat{\mathsf{b}}, \tag{11.4}$$

The guiding-center Hamiltonian, on the other hand, can be chosen as (with $\Pi_{2\|}\equiv 0$)

$$H_{\rm gc} \;=\; \frac{p_{\|}^{2}}{2m} \;+\; J\,\Omega \;+\; \epsilon^{2}\,\Psi_{2}, \tag{11.5}$$

where the second-order guiding-center Hamiltonian is expressed as

$$\Psi_{2} \;=\; J\,\Omega\left(\frac{J}{2\,m\Omega}\,\beta_{2\perp} \;+\; \frac{1}{2}\,\varrho_{\|}^{2}\,\beta_{2\|}\right) \;-\; \frac{p_{\|}^{2}}{2m}\,\left(\varrho_{\|}^{2}\,|\boldsymbol{\kappa}|^{2}\right) \;+\; \mathbf{\Pi}_{1}\boldsymbol{\cdot}\mathbf{v}_{\rm gc}. \tag{11.6}$$

Here, we have isolated the contribution from the perpendicular polarization component $\mathbf{\Pi}_{1\perp}$ and the coefficients $\beta_{2\perp}$ and $\beta_{2\|}$ are defined in Eqs. (7.15)-(7.16).

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, provided $\partial\mathbf{\Pi}_{1}/\partial p_{\|}\equiv 0$. Next, we verified that our guiding-center transformation also satisfy the guiding-center Lagrangian constraints at first and second orders.

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 choice made by Littlejohn in (Littlejohn 1983). We showed in Sec. 10 that the choice $\mathbf{\Pi}_{1} = -\,\frac{1}{2}\,J\;\nabla\times\widehat{\mathsf{b}}$ not only yields the standard Pfirsch-Kaufman guiding-center polarization (10.5) but also an accurate guiding-center representation of the particle toroidal canonical momentum (10.16). By comparison, the guiding-center toroidal canonical momentum obtained by Littlejohn is $(P_{{\rm gc}\varphi})_{\rm RGL} = -\,(e/\epsilon\,c)\,\psi + p_{\|}\,b_{\varphi} - \epsilon\,J\,b_{\mathsf{z}}$ (calculated with the choice $\mathbf{\Pi}_{1\perp}\equiv 0$).

Lastly, we show in App. F, that the guiding-center Hamiltonian (11.5) can be expressed as

$$H_{\rm gc} \;\equiv\; \frac{m}{2}\left\langle\left|\frac{d_{\rm gc}\mathbf{X}}{dt} + \frac{d_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{dt}\right|^{2}\right\rangle. \tag{11.7}$$

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Appendix A. Dyadic Calculus

In this Appendix, we present the basic expressions associated with the gradient and curl operations on the rotating vectors $\widehat{\mathsf{u}}^i \equiv (\widehat{\perp}, \widehat{\rho}, \widehat{\mathsf{b}})$, where we shall use the identities

$$
\begin{aligned}
\mathbf{p}_\perp \times \boldsymbol{\rho}_0 &= 2\,J\,\widehat{\mathsf{b}}, \\
\mathbf{p}_\perp \cdot \frac{\partial \boldsymbol{\rho}_0}{\partial \theta} &= 2\,J \;=\; -\,\frac{\partial \mathbf{p}_\perp}{\partial \theta} \cdot \boldsymbol{\rho}_0, \\
\frac{\partial \mathbf{p}_\perp}{\partial J} \cdot \frac{\partial \boldsymbol{\rho}_0}{\partial \theta} &= 1 \;=\; -\,\frac{\partial \mathbf{p}_\perp}{\partial \theta} \cdot \frac{\partial \boldsymbol{\rho}_0}{\partial J}.
\end{aligned}
$$

In writing the following expressions, we use

$$
\nabla \times \widehat{\mathsf{b}} = \tau\,\widehat{\mathsf{b}} \;+\; \widehat{\mathsf{b}} \times \boldsymbol{\kappa}, \tag{A 1}
$$

$$
\nabla \times \widehat{\perp} = -\,\widehat{\rho} \times \mathbf{R} \;-\; C_{\rho\perp}\,\widehat{\perp} \;+\; C_{\perp\perp}\,\widehat{\rho}, \tag{A 2}
$$

$$
\nabla \times \widehat{\rho} = \widehat{\perp} \times \mathbf{R} \;-\; C_{\rho\rho}\,\widehat{\perp} \;+\; C_{\perp\rho}\,\widehat{\rho}, \tag{A 3}
$$

where the matrix elements

$$
\left.
\begin{aligned}
C_{\perp\perp} &\equiv \widehat{\perp} \cdot \nabla\widehat{\mathsf{b}} \cdot \widehat{\perp} \;=\; \tfrac{1}{2}\,\nabla \cdot \widehat{\mathsf{b}} \;+\; 2\,\alpha_2 \\
C_{\perp\rho} &\equiv \widehat{\perp} \cdot \nabla\widehat{\mathsf{b}} \cdot \widehat{\rho} \;=\; \tfrac{1}{2}\,\tau \;-\; \alpha_1 \\
C_{\rho\perp} &\equiv \widehat{\rho} \cdot \nabla\widehat{\mathsf{b}} \cdot \widehat{\perp} \;=\; -\,\tfrac{1}{2}\,\tau \;-\; \alpha_1 \\
C_{\rho\rho} &\equiv \widehat{\rho} \cdot \nabla\widehat{\mathsf{b}} \cdot \widehat{\rho} \;=\; \tfrac{1}{2}\,\nabla \cdot \widehat{\mathsf{b}} \;-\; 2\,\alpha_2
\end{aligned}
\right\},
\tag{A 4}
$$

with $\alpha_n \equiv \mathsf{a}_n : \nabla\widehat{\mathsf{b}}$ expressed in terms of the dyadic tensors

$$
\mathsf{a}_1 \equiv -\,\frac{1}{2}\left(\widehat{\perp}\,\widehat{\rho} + \widehat{\rho}\,\widehat{\perp}\right) \;=\; \frac{\partial \mathsf{a}_2}{\partial \theta}, \tag{A 5}
$$

$$
\mathsf{a}_2 \equiv \frac{1}{4}\left(\widehat{\perp}\,\widehat{\perp} - \widehat{\rho}\,\widehat{\rho}\right) \;=\; -\,\frac{1}{4}\,\frac{\partial \mathsf{a}_1}{\partial \theta}, \tag{A 6}
$$

so that $\partial\alpha_2/\partial\theta \equiv \alpha_1$ and $\partial\alpha_1/\partial\theta \equiv -\,4\,\alpha_2$.

We also make use of these matrix elements to write the components of the dyadic gradients

$$
\left.
\begin{aligned}
\nabla\widehat{\mathsf{b}} &= \widehat{\mathsf{b}}\,\boldsymbol{\kappa} \;+\; \left(C_{\rho\rho}\,\widehat{\rho}\widehat{\rho} \;+\; C_{\rho\perp}\,\widehat{\rho}\widehat{\perp} \;+\; C_{\perp\rho}\,\widehat{\perp}\widehat{\rho} \;+\; C_{\perp\perp}\,\widehat{\perp}\widehat{\perp}\right) \\
\nabla\widehat{\perp} &= \mathbf{R}\,\widehat{\rho} \;-\; \left(\boldsymbol{\kappa} \cdot \widehat{\perp}\right)\,\widehat{\mathsf{b}}\widehat{\mathsf{b}} \;-\; \left(C_{\perp\perp}\,\widehat{\perp} \;+\; C_{\rho\perp}\,\widehat{\rho}\right)\,\widehat{\mathsf{b}} \\
\nabla\widehat{\rho} &= -\,\mathbf{R}\,\widehat{\perp} \;-\; \left(\boldsymbol{\kappa} \cdot \widehat{\rho}\right)\,\widehat{\mathsf{b}}\widehat{\mathsf{b}} \;-\; \left(C_{\perp\rho}\,\widehat{\perp} \;+\; C_{\rho\rho}\,\widehat{\rho}\right)\,\widehat{\mathsf{b}}
\end{aligned}
\right\},
\tag{A 7}
$$

from which we obtain the divergence identities

$$\left.\begin{array}{rcl} \nabla\cdot\widehat{\mathsf{b}} & = & C_{\rho\rho} \;+\; C_{\perp\perp} \\ \nabla\cdot\widehat{\perp} & = & \mathbf{R}\cdot\widehat{\rho} \;-\; \boldsymbol{\kappa}\cdot\widehat{\perp} \\ \nabla\cdot\widehat{\rho} & = & -\,\mathbf{R}\cdot\widehat{\perp} \;-\; \boldsymbol{\kappa}\cdot\widehat{\rho} \end{array}\right\}, \tag{A 8}$$

and the useful expressions

$$\begin{aligned} \nabla\boldsymbol{\rho}_0 &= -\,\frac{1}{2}\nabla\ln B\;\boldsymbol{\rho}_0 \;-\; \mathbf{R}\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} \;-\; \left[(\boldsymbol{\rho}_0\cdot\boldsymbol{\kappa})\,\widehat{\mathsf{b}} \;+\; C_{\perp\rho}\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} \;+\; C_{\rho\rho}\,\boldsymbol{\rho}_0\right]\widehat{\mathsf{b}}, \\ \nabla\cdot\boldsymbol{\rho}_0 &= -\,\boldsymbol{\rho}_0\cdot\left(\frac{1}{2}\nabla\ln B \;+\; \boldsymbol{\kappa} \;+\; \widehat{\mathsf{b}}\times\mathbf{R}\right), \\ \nabla\times\mathbf{p}_\perp &= \frac{1}{2}\nabla\ln B\times\mathbf{p}_\perp \;-\; \mathbf{R}\times\frac{\partial\mathbf{p}_\perp}{\partial\theta} \;-\; \left(C_{\rho\perp}\,\mathbf{p}_\perp \;+\; C_{\perp\perp}\,\frac{\partial\mathbf{p}_\perp}{\partial\theta}\right), \end{aligned}$$

with

$$\begin{aligned} \langle\boldsymbol{\rho}_0\cdot\nabla\boldsymbol{\rho}_0\rangle &= \frac{J}{m\Omega}\left[\widehat{\mathsf{b}}\times\mathbf{R} \;-\; (\nabla\cdot\widehat{\mathsf{b}})\,\widehat{\mathsf{b}} \;-\; \frac{1}{2}\,\nabla_\perp\ln B\right] \\ \frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\nabla\times\mathbf{p}_\perp &= -\,J\left[2\,\widehat{\mathsf{b}}\cdot\mathbf{R} \;-\; (\tau + 2\,\alpha_1)\right], \\ \frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\nabla\times\frac{\partial\mathbf{p}_\perp}{\partial J} &= -\,\widehat{\mathsf{b}}\cdot\mathbf{R} \;+\; \left(\alpha_1 \;+\; \frac{\tau}{2}\right), \\ \frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\nabla\times\frac{\partial\mathbf{p}_\perp}{\partial\theta} &= -\,4\,J\,\alpha_2. \end{aligned}$$

We will also use the following expressions

$$\begin{aligned} \frac{d_0\boldsymbol{\rho}_0}{dt} &= \frac{p_\parallel}{m}\,\widehat{\mathsf{b}}\cdot\left[\nabla\boldsymbol{\rho}_0 \;+\; \left(\mathbf{R} + \frac{1}{2}\,\nabla\times\widehat{\mathsf{b}}\right)\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right] \\ &= \frac{p_\parallel}{m}\left[\frac{1}{2}\,(\nabla\cdot\widehat{\mathsf{b}})\;\boldsymbol{\rho}_0 \;+\; \frac{1}{2}\,\tau\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} \;-\; (\boldsymbol{\rho}_0\cdot\boldsymbol{\kappa})\;\widehat{\mathsf{b}}\right], \end{aligned} \tag{A 9}$$

$$\begin{aligned} \frac{d_0\mathbf{p}_\perp}{dt} &= \frac{p_\parallel}{m}\,\widehat{\mathsf{b}}\cdot\left[\nabla\mathbf{p}_\perp \;+\; \left(\mathbf{R} + \frac{1}{2}\,\nabla\times\widehat{\mathsf{b}}\right)\frac{\partial\mathbf{p}_\perp}{\partial\theta}\right] \\ &= -\,\frac{p_\parallel}{m}\left[\frac{1}{2}\,(\nabla\cdot\widehat{\mathsf{b}})\;\mathbf{p}_\perp \;-\; \frac{1}{2}\,\tau\,\frac{\partial\mathbf{p}_\perp}{\partial\theta} \;+\; (\mathbf{p}_\perp\cdot\boldsymbol{\kappa})\;\widehat{\mathsf{b}}\right]. \end{aligned} \tag{A 10}$$

We conclude this Appendix by presenting the dyadic identity derived from Eq. (A 7):

$$\begin{aligned} \nabla\widehat{\mathsf{b}} \;:\; \nabla\widehat{\mathsf{b}} &= (C_{\rho\rho})^2 \;+\; (C_{\perp\perp})^2 \;+\; 2\,C_{\perp\rho}\,C_{\rho\perp} \\ &= \frac{1}{2}\left[\left(\nabla\cdot\widehat{\mathsf{b}}\right)^2 \;-\; \tau^2\right] \;+\; 2\left[(\alpha_1)^2 \;+\; 4\;(\alpha_2)^2\right], \end{aligned} \tag{A 11}$$

which implies that

$$(\alpha_1)^2 \;+\; 4\;(\alpha_2)^2 \;\equiv\; \left\langle(\alpha_1)^2\right\rangle \;+\; 4\;\left\langle(\alpha_2)^2\right\rangle, \tag{A 12}$$

as is easily demonstrated by noting that the gyroangle-derivative of the left side of

Eq. (A 12) vanishes. Next, we note that

$$\left\langle (\alpha_1)^2 \right\rangle \;=\; \left\langle \left(\frac{\partial\alpha_2}{\partial\theta}\right)(\alpha_1) \right\rangle \;=\; 4\;\left\langle (\alpha_2)^2 \right\rangle, \tag{A 13}$$

and thus the dyadic identity (A 11) becomes

$$\nabla\widehat{\mathsf{b}}\;:\;\nabla\widehat{\mathsf{b}} \;=\; \nabla\cdot\boldsymbol{\kappa} \;-\; \widehat{\mathsf{b}}\cdot\nabla(\nabla\cdot\widehat{\mathsf{b}}) \;=\; \frac{1}{2}\left[\left(\nabla\cdot\widehat{\mathsf{b}}\right)^2 \;-\; \tau^2\right] \;+\; 4\;\left\langle (\alpha_1)^2 \right\rangle. \tag{A 14}$$

We will also need the related dyadic identity

$$\begin{aligned}(\nabla\widehat{\mathsf{b}})^\top \;:\; \nabla\widehat{\mathsf{b}} &= |\boldsymbol{\kappa}|^2 + (C_{\rho\rho})^2 + (C_{\perp\perp})^2 + (C_{\perp\rho})^2 + (C_{\rho\perp})^2 \\ &= |\boldsymbol{\kappa}|^2 + \frac{1}{2}\left[\left(\nabla\cdot\widehat{\mathsf{b}}\right)^2 + \tau^2\right] + 4\;\left\langle (\alpha_1)^2 \right\rangle \;=\; \nabla\widehat{\mathsf{b}}\;:\;\nabla\widehat{\mathsf{b}} + |\boldsymbol{\kappa}|^2 + \tau^2.\end{aligned} \tag{A 15}$$

Lastly, we give the expression for the gyrogauge-invariant vector field

$$\nabla\times\mathbf{R} = \frac{1}{2}\left[\nabla\widehat{\mathsf{b}}:\nabla\widehat{\mathsf{b}} \;-\; (\nabla\cdot\widehat{\mathsf{b}})^2\right]\;\widehat{\mathsf{b}} \;+\; (\nabla\cdot\widehat{\mathsf{b}})\;\boldsymbol{\kappa} \;-\; \boldsymbol{\kappa}\cdot\nabla\widehat{\mathsf{b}}, \tag{A 16}$$

which yields the relations

$$\widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} \;=\; \frac{1}{2}\;\nabla\cdot\;\left[\boldsymbol{\kappa} \;-\; \widehat{\mathsf{b}}\,(\nabla\cdot\widehat{\mathsf{b}})\right], \tag{A 17}$$

and

$$\langle\alpha_1^2\rangle \;=\; \frac{1}{2}\,\widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} \;+\; \frac{1}{8}\left[\tau^2 \;+\; \left(\nabla\cdot\widehat{\mathsf{b}}\right)^2\right]. \tag{A 18}$$

Appendix B. Calculations of D_1 and D_1^2

We begin with the operators D_1 and D_1^2 acting on $p_\| \,\widehat{\mathsf{b}}$:

$$D_1\left(p_\|\,\widehat{\mathsf{b}}\right) = \left(G_1^{p_\|} \;+\; p_\|\;\boldsymbol{\rho}_0\cdot\boldsymbol{\kappa}\right)\widehat{\mathsf{b}} \;+\; p_\|\;\tau\;\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} \;=\; J\;\left(\tau \;+\; \alpha_1\right)\;\widehat{\mathsf{b}} \;+\; \varrho_\|\,\tau\;\mathbf{p}_\perp, \tag{B 1}$$

$$\begin{aligned}D_1^2\left(p_\|\,\widehat{\mathsf{b}}\right) = &\left[J\,\tau\,(\tau+\alpha_1) \;+\; \tau\left(G_1^{p_\|} \;+\; \frac{p_\|}{2J}\,G_1^J\right) \;+\; \varrho_\| B\,\widehat{\mathsf{b}}\cdot\nabla\times\;\left(\frac{\tau}{B}\;\mathbf{p}_\perp\right)\right]\;\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} \\ &-\;\left(p_\|\,\tau\,G_1^\theta\right)\boldsymbol{\rho}_0 \;+\; \left[G_1^J\;(\tau+\alpha_1) \;-\; 4\,J\,\alpha_2\,G_1^\theta \;-\; \varrho_\|\,\tau\;\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\nabla\times\mathbf{p}_\perp\right. \\ &\left.-\;J\;\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\nabla\times\;\left[(\tau+\alpha_1)\,\widehat{\mathsf{b}}\right]\right]\;\widehat{\mathsf{b}},\end{aligned} \tag{B 2}$$

from which we obtain

$$\left.\begin{aligned}\langle D_1(p_\|\,\widehat{\mathsf{b}})\rangle &= J\,\tau\,\widehat{\mathsf{b}} \\ D_1(p_\|\,\widehat{\mathsf{b}})\cdot\boldsymbol{\rho}_0 &= 0 \\ D_1(p_\|\,\widehat{\mathsf{b}})\cdot\partial\boldsymbol{\rho}_0/\partial\theta &= 2\,J\;\varrho_\|\,\tau\end{aligned}\right\}, \tag{B 3}$$

and

$$\left\langle D_1^2\left(p_\| \,\widehat{\mathsf{b}}\right)\right\rangle\cdot\widehat{\mathsf{b}} = \left\langle G_1^J\,(\tau+\alpha_1)\;-\;4\,J\,\alpha_2 G_1^\theta\right\rangle\;-\;\varrho_\|\,\tau\;\left\langle\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\nabla\times\mathbf{p}_\perp\right\rangle$$
$$= -\,2\,J\,\varrho_\|\left(\tau^2\;+\;\langle\alpha_1^2\rangle\;-\;\tau\,\widehat{\mathsf{b}}\cdot\mathbf{R}\right), \quad \text{(B 4)}$$

$$\left\langle D_1^2\left(p_\|\,\widehat{\mathsf{b}}\right)\cdot\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right\rangle = \frac{2J}{m\Omega}\left(J\,\tau^2+\tau\left\langle G_1^{p_\|}+\frac{p_\|}{2J}\,G_1^J\right\rangle\right) = \left(\frac{4\,J^2}{m\Omega}-J\,\varrho_\|^2\right)\tau^2, \quad \text{(B 5)}$$

$$\left\langle D_1\left(p_\|\,\widehat{\mathsf{b}}\right)\cdot\frac{\partial G_2^{\mathbf{x}}}{\partial\theta}\right\rangle = J\left\langle\alpha_1\,\frac{\partial G_{2\|}^{\mathbf{x}}}{\partial\theta}\right\rangle\;+\;\varrho_\|\tau\;\left(2\,J\,\varrho_\|\tau\;+\;\frac{1}{2}\,\langle g_1^J\rangle\right)$$
$$= \frac{J^2}{m\Omega}\,\langle\alpha_1^2\rangle\;+\;\frac{3}{2}\,J\,\varrho_\|^2\tau^2. \quad \text{(B 6)}$$

Next, we consider the operators D_1 and D_1^2 acting on $\mathbf{p}_\perp$:

$$D_1(\mathbf{p}_\perp) = \mathsf{G}_1\cdot\mathsf{d}\mathbf{p}_\perp\;+\;2\,J\,\mathbf{R}\;=\;J\left[2\,\mathbf{R}\;-\;(\tau+2\,\alpha_1)\,\widehat{\mathsf{b}}\right]\;+\;g_1^J\,\frac{\partial\mathbf{p}_\perp}{\partial J}\;+\;g_1^\theta\,\frac{\partial\mathbf{p}_\perp}{\partial\theta}$$
$$= J\left[2\,\mathbf{R}\;-\;(\tau+2\,\alpha_1)\,\widehat{\mathsf{b}}\right]\;+\;\left[\frac{p_\|^2}{m\Omega}\,(\boldsymbol{\rho}_0\cdot\boldsymbol{\kappa})\;-\;J\,\varrho_\|\,(\tau+\alpha_1)\right]\frac{\partial\mathbf{p}_\perp}{\partial J}$$
$$+\;\left[\varrho_\|\alpha_2\;+\;\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\left(\nabla\ln B\;+\;\frac{p_\|^2\,\boldsymbol{\kappa}}{2m\Omega\,J}\right)\right]\frac{\partial\mathbf{p}_\perp}{\partial\theta}, \quad \text{(B 7)}$$

$$D_1^2(\mathbf{p}_\perp) = 2\,G_1^J\,\mathbf{R}\;-\;\left[G_1^J\,\left(\tau\;+\;2\,\alpha_1\right)\;-\;8\,J\alpha_2\,G_1^\theta\right]\,\widehat{\mathsf{b}}\;+\;\boldsymbol{\rho}_0\times\nabla\times\left[D_1(\mathbf{p}_\perp)\right]$$
$$+\;\left[\left(G_1^a\,\partial_a g_1^J\right)-2\,J\,g_1^\theta\,G_1^\theta-\frac{1}{2J}\,g_1^J\,G_1^J\right]\frac{\partial\mathbf{p}_\perp}{\partial J}$$
$$+\;\left[\left(G_1^a\,\partial_a g_1^\theta\right)+\frac{1}{2J}\left(g_1^J\,G_1^\theta+g_1^\theta\,G_1^J\right)\right]\frac{\partial\mathbf{p}_\perp}{\partial\theta}, \quad \text{(B 8)}$$

from which we obtain

$$\left.\begin{array}{rcl}\langle D_1(\mathbf{p}_\perp)\rangle & = & J\,(2\mathbf{R}-\tau\,\widehat{\mathsf{b}})\;-\;\widehat{\mathsf{b}}\times(J\,\nabla\ln B+p_\|\,\varrho_\|\,\boldsymbol{\kappa})\\ D_1(\mathbf{p}_\perp)\cdot\boldsymbol{\rho}_0 & = & -\,2\,J\,G_1^\theta\\ D_1(\mathbf{p}_\perp)\cdot\partial\boldsymbol{\rho}_0/\partial\theta & = & 2\,J\,\mathbf{R}\cdot\partial\boldsymbol{\rho}_0/\partial\theta+(G_1^J-J\,\boldsymbol{\rho}_0\cdot\nabla\ln B)\end{array}\right\}, \quad \text{(B 9)}$$

and

$$\left\langle D_1^2(\mathbf{p}_\perp)\right\rangle \cdot \widehat{\mathsf{b}} = 2\,\langle G_1^J\rangle\,\widehat{\mathsf{b}}\cdot\mathbf{R} \;-\; \left\langle G_1^J\;(\tau + 2\,\alpha_1) \;-\; 8\,J\alpha_2\;G_1^\theta\right\rangle$$
$$-\;\left\langle \frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\nabla\times[D_1(\mathbf{p}_\perp)]\right\rangle$$
$$= J\,\varrho_\parallel\left(\frac{3}{2}\,\tau^2 \;+\; 6\,\langle\alpha_1^2\rangle \;-\; 3\,\tau\,\widehat{\mathsf{b}}\cdot\mathbf{R}\right), \tag{B 10}$$

$$\left\langle D_1^2(\mathbf{p}_\perp)\cdot\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right\rangle = 2\left\langle G_1^J\,\boldsymbol{\rho}_0\right\rangle\cdot\widehat{\mathsf{b}}\times\mathbf{R} + 2\,J\,\frac{\widehat{\mathsf{b}}}{m\Omega}\cdot\nabla\times\,\langle D_1(\mathbf{p}_\perp)\rangle$$
$$+\;\left\langle \left(G_1^a\,\partial_a g_1^J\right) - 2\,J\,g_1^\theta\,G_1^\theta - \frac{1}{2J}\,g_1^J\,G_1^J\right\rangle, \tag{B 11}$$

$$\left\langle D_1(\mathbf{p}_\perp)\cdot\frac{\partial G_2^{\mathbf{x}}}{\partial\theta}\right\rangle = -\,\frac{2\,J^2}{m\Omega}\,\langle\alpha_1^2\rangle \;-\; J\,\varrho_\parallel^2\,\tau^2$$
$$+\;\left\langle J\;\left(g_1^\theta\right)^2 \;+\; \frac{1}{4J}\;\left(g_1^J\right)^2 \;+\; g_1^J\,\frac{\partial g_1^\theta}{\partial\theta}\right\rangle, \tag{B 12}$$

where

$$\widehat{\mathsf{b}}\cdot\nabla\times\langle D_1(\mathbf{p}_\perp)\rangle = 2\,J\,\widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} \;-\; J\,\tau^2 \;-\; \widehat{\mathsf{b}}\cdot\nabla\times\left[\widehat{\mathsf{b}}\times\left(J\,\nabla\ln B \;+\; \frac{p_\parallel^2\,\boldsymbol{\kappa}}{m\Omega}\right)\right],$$

$$\left\langle\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\nabla\times[D_1(\mathbf{p}_\perp)]\right\rangle = \left\langle\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\nabla\times\left(g_1^J\,\frac{\partial\mathbf{p}_\perp}{\partial J} \;+\; g_1^\theta\,\frac{\partial\mathbf{p}_\perp}{\partial\theta}\right)\right\rangle$$
$$= -\,J\,\varrho_\parallel\;\left(\frac{\tau^2}{2} \;+\; 2\,\langle\alpha_1^2\rangle \;-\; \tau\,\widehat{\mathsf{b}}\cdot\mathbf{R}\right).$$

Lastly, we need

$$F_{1p_\parallel} \;=\; \frac{\partial D_1(\mathbf{P}_4)}{\partial p_\parallel}\cdot\boldsymbol{\rho}_0 = -\,\frac{1}{2}\,J\,\frac{\partial g_1^\theta}{\partial p_\parallel}, \tag{B 13}$$

$$F_{1J} \;=\; \frac{\partial D_1(\mathbf{P}_4)}{\partial J}\cdot\boldsymbol{\rho}_0 = -\,\frac{1}{2}\left(J\,\frac{\partial g_1^\theta}{\partial J} \;+\; \frac{1}{2}\,g_1^\theta\right) \;+\; \frac{1}{2}\,\boldsymbol{\rho}_0\cdot\mathbf{R}, \tag{B 14}$$

$$F_{1\theta} \;=\; \frac{\partial D_1(\mathbf{P}_4)}{\partial\theta}\cdot\boldsymbol{\rho}_0 = -\,\frac{1}{2}\left(J\,\frac{\partial g_1^\theta}{\partial\theta} \;+\; \frac{1}{2}\,g_1^J\right) \;-\; \frac{2}{3}\,J\,\varrho_\parallel\tau, \tag{B 15}$$

and

$$\frac{\partial F_{1\theta}}{\partial p_\parallel} \;-\; \frac{\partial F_{1p_\parallel}}{\partial\theta} = -\,\frac{1}{4}\,\frac{\partial g_1^J}{\partial p_\parallel} \;-\; \frac{2}{3}\,\frac{J\tau}{m\Omega}, \tag{B 16}$$

$$\frac{\partial F_{1\theta}}{\partial J} \;-\; \frac{\partial F_{1J}}{\partial\theta} = -\,\frac{1}{4}\left(\frac{\partial g_1^J}{\partial J} \;+\; \frac{\partial g_1^\theta}{\partial\theta}\right) \;-\; \frac{1}{2}\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\mathbf{R} \;-\; \frac{2}{3}\,\varrho_\parallel\tau. \tag{B 17}$$

Appendix C. Second-order Calculations for $\langle G_2^J\rangle$

Equation (7.12) defines the gyroangle-averaged component $\langle G_2^J\rangle$:

$$\langle G_2^J\rangle = \frac{1}{2}\left\langle\frac{\partial G_2^{\mathbf{x}}}{\partial\theta}\cdot D_1(\mathbf{P}_2)\right\rangle \;+\; \frac{1}{4}\left\langle G_1^J\,\frac{\partial G_1^\theta}{\partial\theta} \;-\; G_1^\theta\,\frac{\partial G_1^J}{\partial\theta} \;+\; \mathsf{G}_1\cdot\mathsf{d}G_1^J\right\rangle$$
$$+\;\frac{1}{2}\left\langle\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot D_1^2(\mathbf{P}_4)\right\rangle \;-\; \frac{1}{2}\left\langle\mathsf{G}_1\cdot\mathsf{d}F_{1\theta} \;-\; G_1^a\,\frac{\partial F_{1a}}{\partial\theta}\right\rangle, \tag{C 1}$$

where

$$\frac{\partial G_2^{\mathbf{x}}}{\partial\theta} = \left(\frac{J\,\alpha_1}{m\Omega} \;-\; 2\,\varrho_\parallel\,\boldsymbol{\rho}_0\cdot\boldsymbol{\kappa}\right)\widehat{\mathsf{b}} \;+\; \varrho_\parallel\,\tau\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} \;+\; \frac{1}{2}\left(\frac{\partial g_1^J}{\partial\theta} \;-\; 2J\,g_1^\theta\right)\frac{\partial\boldsymbol{\rho}_0}{\partial J} + \frac{1}{2}\left(\frac{\partial g_1^\theta}{\partial\theta} \;+\; \frac{1}{2J}\,g_1^J\right)\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}, \tag{C 2}$$

where $g_1^J \equiv G_1^J - J\;\boldsymbol{\rho}_0\cdot\nabla\ln B$ and $g_1^\theta \equiv G_1^\theta + \boldsymbol{\rho}_0\cdot\mathbf{R}$. We now compute each term respectively. The first and third terms are

$$\frac{1}{2}\left\langle\frac{\partial G_2^{\mathbf{x}}}{\partial\theta}\cdot D_1(\mathbf{P}_2)\right\rangle = \frac{1}{2}\,J\,\varrho_\parallel^2\,\tau^2 \;+\; \frac{1}{4}\left\langle J\;\left(g_1^\theta\right)^2 \;+\; \frac{1}{4J}\;\left(g_1^J\right)^2 \;+\; g_1^J\,\frac{\partial g_1^\theta}{\partial\theta}\right\rangle, \tag{C 3}$$

$$\begin{aligned}\frac{1}{2}\left\langle\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot D_1^2(\mathbf{P}_4)\right\rangle = {}& \left(\frac{2\,J^2}{3\,m\Omega} \;-\; \frac{1}{2}\,J\,\varrho_\parallel^2\right)\tau^2 \;+\; \frac{1}{4}\left\langle\left(G_1^J \;+\; \frac{1}{2}g_1^J\right)\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} \;+\; J\,g_1^\theta\,\boldsymbol{\rho}_0\right\rangle\cdot\mathbf{R} \\ &+ \frac{J\,\widehat{\mathsf{b}}}{4\,m\Omega}\cdot\nabla\times\langle D_1(\mathbf{p}_\perp)\rangle \;-\; \frac{1}{4}\left\langle J\;\left(g_1^\theta\right)^2 \;+\; \frac{1}{4J}\;\left(g_1^J\right)^2\right\rangle \\ &+ \frac{1}{8}\left\langle G_1^{p_\parallel}\,\frac{\partial g_1^J}{\partial p_\parallel} \;+\; G_1^J\,\frac{\partial g_1^J}{\partial J} \;-\; g_1^J\left(\frac{1}{2}\,\boldsymbol{\rho}_0\cdot\nabla\ln B \;+\; \frac{\partial g_1^\theta}{\partial\theta}\right)\right\rangle,\end{aligned} \tag{C 4}$$

while the second and fourth terms are

$$\begin{aligned}\frac{1}{4}\left\langle G_1^J\,\frac{\partial G_1^\theta}{\partial\theta} \;-\; G_1^\theta\,\frac{\partial G_1^J}{\partial\theta} \;+\; \mathsf{G}_1\cdot\mathsf{d}G_1^J\right\rangle = {}& -\,\frac{1}{4}\;\left\langle G_1^J\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right\rangle\cdot\mathbf{R} \;+\; \frac{1}{4}\left\langle G_1^{p_\parallel}\,\frac{\partial g_1^J}{\partial p_\parallel}\right\rangle \\ &-\,\frac{1}{4}\;\left\langle\boldsymbol{\rho}_0\;\cdot\nabla G_1^J\right\rangle \\ &+\frac{1}{4}\left\langle G_1^J\left(\frac{3}{2}\,\boldsymbol{\rho}_0\cdot\nabla\ln B \;+\; \frac{\partial g_1^J}{\partial J} \;+\; \frac{\partial g_1^\theta}{\partial\theta}\right)\right\rangle,\end{aligned} \tag{C 5}$$

and

$$\begin{aligned}-\,\frac{1}{2}\left\langle\mathsf{G}_1\cdot\mathsf{d}F_{1\theta} \;-\; G_1^a\,\frac{\partial F_{1a}}{\partial\theta}\right\rangle = {}& -\,\frac{1}{4}\left\langle\boldsymbol{\rho}_0\cdot\nabla\left(J\,\frac{\partial g_1^\theta}{\partial\theta} \;+\; \frac{1}{2}\,g_1^J\right)\right\rangle \\ &+\frac{1}{4}\;\left\langle G_1^J\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right\rangle\cdot\mathbf{R} + \frac{1}{3}\left\langle G_1^{p_\parallel}\,\frac{J\tau}{m\Omega} \;+\; G_1^J\,\varrho_\parallel\,\tau\right\rangle \\ &+\frac{1}{8}\left\langle G_1^{p_\parallel}\,\frac{\partial g_1^J}{\partial p_\parallel} \;+\; G_1^J\left(\frac{\partial g_1^J}{\partial J} \;+\; \frac{\partial g_1^\theta}{\partial\theta}\right)\right\rangle,\end{aligned} \tag{C 6}$$

so that Eq. (C 1) becomes

$$\begin{aligned}\langle G_2^J\rangle = {}& \frac{1}{3}\left[\left(\frac{2J^2}{m\Omega} \;+\; J\,\varrho_\parallel^2\right)\tau^2 \;+\; \left\langle G_1^{p_\parallel}\,\frac{J\,\tau}{m\Omega} \;+\; G_1^J\,\varrho_\parallel\,\tau\right\rangle\right] \;+\; \frac{1}{2}\;\left\langle G_1^{p_\parallel}\,\frac{\partial g_1^J}{\partial p_\parallel}\right\rangle \\ &+ \frac{J\,\widehat{\mathsf{b}}}{4\,m\Omega}\cdot\nabla\times\langle D_1(\mathbf{p}_\perp)\rangle + \frac{1}{4}\;\left\langle\left(G_1^J \;+\; \frac{1}{2}\,g_1^J\right)\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} \;+\; J\,g_1^\theta\,\boldsymbol{\rho}_0\right\rangle\cdot\mathbf{R} \\ &-\frac{1}{4}\left\langle\boldsymbol{\rho}_0\cdot\nabla\left(G_1^J \;+\; \frac{1}{2}\,g_1^J \;+\; J\,\frac{\partial g_1^\theta}{\partial\theta}\right)\right\rangle \\ &+\frac{1}{4}\left\langle G_1^J\left[\frac{3}{2}\left(\boldsymbol{\rho}_0\cdot\nabla\ln B + \frac{\partial g_1^\theta}{\partial\theta}\right) + 2\,\frac{\partial g_1^J}{\partial J}\right] + \frac{1}{2}\,g_1^J\left(\frac{\partial g_1^\theta}{\partial\theta} - \frac{1}{2}\,\boldsymbol{\rho}_0\cdot\nabla\ln B\right)\right\rangle.\end{aligned} \tag{C 7}$$

We now use the identity $\boldsymbol{\rho}_0\cdot\nabla A = \nabla\cdot(\boldsymbol{\rho}_0\, A) - A\,(\nabla\cdot\boldsymbol{\rho}_0)$, where

$$\nabla\cdot\boldsymbol{\rho}_0 \;=\; -\,\boldsymbol{\rho}_0\cdot\left(\frac{1}{2}\nabla\ln B \;+\; \boldsymbol{\kappa}\right) \;-\; \frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\mathbf{R},$$

so that we obtain

$$\begin{aligned}
-\,\frac{1}{4}\left\langle\boldsymbol{\rho}_0\cdot\nabla\left(G_1^J \;+\; \frac{1}{2}\,g_1^J \;+\; J\,\frac{\partial g_1^\theta}{\partial\theta}\right)\right\rangle \\
&= -\,\frac{1}{4}\nabla\cdot\left\langle\boldsymbol{\rho}_0\,\left(G_1^J \;+\; \frac{1}{2}\,g_1^J \;+\; J\,\frac{\partial g_1^\theta}{\partial\theta}\right)\right\rangle \\
&\quad -\,\frac{1}{4}\left\langle\left(G_1^J \;+\; \frac{1}{2}\,g_1^J\right)\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} \;+\; J\,g_1^\theta\,\boldsymbol{\rho}_0\right\rangle\cdot\mathbf{R} \\
&\quad -\,\frac{1}{4}\left\langle\left(G_1^J \;+\; \frac{1}{2}\,g_1^J \;+\; J\,\frac{\partial g_1^\theta}{\partial\theta}\right)\boldsymbol{\rho}_0\cdot\left(\frac{1}{2}\nabla\ln B \;+\; \boldsymbol{\kappa}\right)\right\rangle. \qquad \text{(C 8)}
\end{aligned}$$

By substituting this expression into Eq. (C 7), we obtain

$$\begin{aligned}
\langle G_2^J\rangle = \frac{1}{3}\left[\left(\frac{2J^2}{m\Omega} \;+\; J\,\varrho_\|^2\right)\tau^2 \;+\; \left\langle G_1^{p_\|}\,\frac{J\,\tau}{m\Omega} \;+\; G_1^J\,\varrho_\|\,\tau\right\rangle\right] \\
+\;\frac{J\,\widehat{\mathsf{b}}}{4\,m\Omega}\cdot\nabla\times\langle D_1(\mathbf{p}_\perp)\rangle \;+\; \frac{1}{2}\,\left\langle G_1^{p_\|}\,\frac{\partial g_1^J}{\partial p_\|}\right\rangle \\
-\;\frac{1}{4}\nabla\cdot\left\langle\boldsymbol{\rho}_0\,\left(G_1^J \;+\; \frac{1}{2}\,g_1^J \;+\; J\,\frac{\partial g_1^\theta}{\partial\theta}\right)\right\rangle \\
+\;\frac{1}{4}\left\langle G_1^J\left[\boldsymbol{\rho}_0\cdot\left(\nabla\ln B \;-\; \boldsymbol{\kappa}\right) \;+\; \frac{3}{2}\,\frac{\partial g_1^\theta}{\partial\theta} \;+\; 2\,\frac{\partial g_1^J}{\partial J}\right]\right\rangle \\
+\;\frac{1}{8}\,\left\langle g_1^J\left[\frac{\partial g_1^\theta}{\partial\theta} \;-\; \boldsymbol{\rho}_0\cdot\left(\nabla\ln B \;+\; \boldsymbol{\kappa}\right)\right]\right\rangle \\
-\;\frac{J}{4}\,\left\langle\frac{\partial g_1^\theta}{\partial\theta}\,\boldsymbol{\rho}_0\cdot\left(\frac{1}{2}\nabla\ln B \;+\; \boldsymbol{\kappa}\right)\right\rangle. \qquad \text{(C 9)}
\end{aligned}$$

We now substitute the definitions of the generating vector-field components and we obtain

$$\begin{aligned}
\langle G_2^J\rangle = \frac{J^2}{2m\Omega}\left[\frac{1}{2}\,\tau^2 \;+\; \widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} \;-\; \langle\alpha_1^2\rangle \;-\; \frac{1}{2}\,\widehat{\mathsf{b}}\cdot\nabla\times\,\left(\widehat{\mathsf{b}}\times\nabla\ln B\right)\right] \\
-\;\frac{1}{2}\,J\,\varrho_\|^2\left[\boldsymbol{\kappa}\cdot(3\,\boldsymbol{\kappa} - \nabla\ln B) \;+\; \nabla\cdot\boldsymbol{\kappa} \;-\; \tau^2\right]. \qquad \text{(C 10)}
\end{aligned}$$

Appendix D. Calculation Details for $(p_\|/m)\,\Pi_{2\|} - \Psi_2$

The defining equation

$$\begin{aligned}
m\,\frac{\partial}{\partial p_\|}\left(\frac{p_\|}{m}\,\Pi_{2\|} \;-\; \Psi_2\right) = m\,\frac{d_0\langle\boldsymbol{\rho}_1\rangle}{dt}\cdot\widehat{\mathsf{b}} \;+\; p_\|\,\boldsymbol{\kappa}\cdot\langle G_2^{\mathbf{x}}\rangle \;-\; \left\langle G_2^{\mathbf{x}}\cdot\nabla\widehat{\mathsf{b}}\cdot\mathbf{p}_\perp\right\rangle \\
+\;\widehat{\mathsf{b}}\cdot\,\left\langle D_1^2(\mathbf{P}_3)\right\rangle \;-\; \frac{1}{2}\left\langle\mathsf{G}_1\cdot\,\mathsf{d}\,(\mathsf{G}_1\cdot\mathsf{d}\mathbf{p})\right\rangle\cdot\widehat{\mathsf{b}} \qquad \text{(D 1)}
\end{aligned}$$

contains five terms that are calculated explicitly in this Appendix. The first term is

$$m\,\frac{d_0\langle\boldsymbol{\rho}_1\rangle}{dt}\cdot\widehat{\mathsf{b}} = \left(p_\parallel\,\widehat{\mathsf{b}}\cdot\nabla\langle\boldsymbol{\rho}_1\rangle\right)\cdot\widehat{\mathsf{b}} \;=\; p_\parallel\,\widehat{\mathsf{b}}\cdot\nabla\left(\langle\boldsymbol{\rho}_1\rangle\cdot\widehat{\mathsf{b}}\right) \;-\; p_\parallel\,\langle\boldsymbol{\rho}_1\rangle\cdot\boldsymbol{\kappa}$$
$$= -\,\frac{1}{2}\,J\,\varrho_\parallel\,\left\{\nabla\cdot\left[\widehat{\mathsf{b}}\,\left(\nabla\cdot\widehat{\mathsf{b}}\right)\right] \;-\; 3\,\boldsymbol{\kappa}\cdot\nabla\ln B\right\} \;+\; p_\parallel\,\varrho_\parallel^2|\boldsymbol{\kappa}|^2$$
$$-\;\varrho_\parallel\,\widehat{\mathsf{b}}\times\boldsymbol{\kappa}\cdot\boldsymbol{\Pi}_1, \tag{D 2}$$

where $\partial(\langle\boldsymbol{\rho}_1\rangle\cdot\widehat{\mathsf{b}})/\partial p_\parallel = 0$ follows from Eq. (10.3). The second term in Eq. (D 1) is

$$p_\parallel\,\langle G_2^{\mathbf{x}}\rangle\cdot\boldsymbol{\kappa} \;=\; -\,\varrho_\parallel\,\widehat{\mathsf{b}}\times\boldsymbol{\kappa}\cdot\boldsymbol{\Pi}_1 \;+\; \frac{1}{2}\,\left(J\,\varrho_\parallel\,\boldsymbol{\kappa}\cdot\nabla\ln B \;+\; p_\parallel\,\varrho_\parallel^2|\boldsymbol{\kappa}|^2\right), \tag{D 3}$$

where we substituted Eq. (6.24). The third term in Eq. (D 1) is

$$-\,\left\langle G_2^{\mathbf{x}}\cdot\nabla\widehat{\mathsf{b}}\cdot\mathbf{p}_\perp\right\rangle = -\,\left\langle G_2^{\mathbf{x}}\cdot\left[\widehat{\mathsf{b}}\,(\boldsymbol{\kappa}\cdot\mathbf{p}_\perp) \;-\; C_{\rho\perp}\,\frac{\partial\mathbf{p}_\perp}{\partial\theta} \;+\; C_{\perp\perp}\,\mathbf{p}_\perp\right]\right\rangle \tag{D 4}$$
$$= -\,\boldsymbol{\kappa}\cdot\left\langle\mathbf{p}_\perp\,G_{2\parallel}^{\mathbf{x}}\right\rangle \;-\; 2\,J\,(\varrho_\parallel\,\tau)\,\langle C_{\rho\perp}\rangle$$
$$-\;\frac{1}{2}\,\left\langle C_{\rho\perp}\,\left(G_1^J - J\,\boldsymbol{\rho}_0\cdot\nabla\ln B\right)\right\rangle \;-\; J\,\left\langle C_{\perp\perp}\,\left(G_1^\theta \;+\; \boldsymbol{\rho}_0\cdot\mathbf{R}\right)\right\rangle,$$

Here, using Eq. (6.20), we find $-\,\langle G_{2\parallel}^{\mathbf{x}}\,\mathbf{p}_\perp\rangle\cdot\boldsymbol{\kappa} = -\,2\,J\,\varrho_\parallel\,|\boldsymbol{\kappa}|^2$, using Eq. (A 7), we find $-\,2\,J\,(\varrho_\parallel\,\tau)\,\langle C_{\rho\perp}\rangle = J\,\varrho_\parallel\,\tau^2$, while using Eqs. (6.17) and (6.21), we obtain

$$-\,\frac{1}{2}\,\left\langle C_{\rho\perp}\,\left(G_1^J - J\,\boldsymbol{\rho}_0\cdot\nabla\ln B\right)\right\rangle \;=\; -\,\frac{1}{2}\,J\,\varrho_\parallel\left(\frac{1}{2}\,\tau^2 + \langle\alpha_1^2\rangle\right),$$

and

$$-\,J\left\langle C_{\perp\perp}\,\left(G_1^\theta + \boldsymbol{\rho}_0\cdot\mathbf{R}\right)\right\rangle \;=\; -\,2\,J\,\varrho_\parallel\,\langle\alpha_2^2\rangle \;\equiv\; -\,\frac{1}{2}\,J\,\varrho_\parallel\,\langle\alpha_1^2\rangle,$$

so that Eq. (D 3) becomes

$$-\,\left\langle G_2^{\mathbf{x}}\cdot\nabla\widehat{\mathsf{b}}\cdot\mathbf{p}_\perp\right\rangle \;=\; J\,\varrho_\parallel\left(\frac{3}{4}\,\tau^2 \;-\; 2\,|\boldsymbol{\kappa}|^2 \;-\; \langle\alpha_1^2\rangle\right), \tag{D 5}$$

where

$$\langle\alpha_1^2\rangle \;\equiv\; \frac{1}{4}\,\nabla\widehat{\mathsf{b}}:\nabla\widehat{\mathsf{b}} \;+\; \frac{1}{8}\left[\tau^2 \;-\; (\nabla\cdot\widehat{\mathsf{b}})^2\right] \;\equiv\; 4\,\langle\alpha_2^2\rangle. \tag{D 6}$$

For the fourth term in Eq. (D 1), we use Eq. (6.28):

$$\widehat{\mathsf{b}}\cdot\,\langle D_1^2(\mathbf{P}_3)\rangle \;=\; -\,J\,\varrho_\parallel\left(\frac{1}{2}\,\tau^2 \;-\; \langle\alpha_1^2\rangle\right). \tag{D 7}$$

Lastly, for the fifth term in Eq. (D 1), we begin with the identity

$$\left\langle\mathsf{G}_1\cdot\,\mathsf{d}\,(\mathsf{G}_1\cdot\mathsf{d}\mathbf{p})\right\rangle\cdot\widehat{\mathsf{b}} \;\equiv\; \left\langle\mathsf{G}_1\cdot\mathsf{d}\left[(\mathsf{G}_1\cdot\mathsf{d}\mathbf{p})\cdot\,\widehat{\mathsf{b}}\right]\right\rangle \;+\; \left\langle\boldsymbol{\rho}_0\cdot\nabla\widehat{\mathsf{b}}\cdot\,(\mathsf{G}_1\cdot\mathsf{d}\mathbf{p})\right\rangle,$$

where

$$\mathsf{G}_1\cdot\mathsf{d}\mathbf{p} = \left(G_1^{p_\parallel} \;+\; 2\,J\,C_{\rho\perp}\right)\,\widehat{\mathsf{b}} \;+\; \left(G_1^J \;-\; J\,\boldsymbol{\rho}_0\cdot\nabla\ln B\right)\frac{\partial\mathbf{p}_\perp}{\partial J}$$
$$+\;\left(G_1^\theta \;+\; \boldsymbol{\rho}_0\cdot\mathbf{R}\right)\frac{\partial\mathbf{p}_\perp}{\partial\theta} \;-\; p_\parallel\,\boldsymbol{\rho}_0\cdot\nabla\widehat{\mathsf{b}}, \tag{D 8}$$

with

$$\boldsymbol{\rho}_0\cdot\nabla\widehat{\mathsf{b}} \;\equiv\; C_{\rho\rho}\,\boldsymbol{\rho}_0 \;+\; C_{\rho\perp}\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}.$$

First, we find

$$-\frac{1}{2}\left\langle \mathsf{G}_1\cdot\mathsf{d}\left[(\mathsf{G}_1\cdot\mathsf{d}\mathbf{p})\cdot\,\widehat{\mathsf{b}}\right]\right\rangle = \frac{1}{2}\left\langle G_1^{p_\|}\;\boldsymbol{\rho}_0\cdot\boldsymbol{\kappa} \;+\; G_1^J\,\alpha_1 \;+\; J\,G_1^\theta\,\frac{\partial\alpha_1}{\partial\theta}\right\rangle$$
$$+\,p_\|\left(\boldsymbol{\kappa}\cdot\left\langle\frac{1}{2}\,\mathsf{G}_1\cdot\mathsf{d}\boldsymbol{\rho}_0\right\rangle \;-\;\frac{1}{2}\left\langle\boldsymbol{\rho}_0\cdot\nabla\boldsymbol{\kappa}\cdot\boldsymbol{\rho}_0\right\rangle\right), \tag{D 9}$$

where we used $(\mathsf{G}_1\cdot\mathsf{d}\mathbf{p})\cdot\widehat{\mathsf{b}} = G_1^{p_\|} + 2\,J\,C_{\rho\perp} = -\,p_\|\,\boldsymbol{\rho}_0\cdot\boldsymbol{\kappa} - J\,\alpha_1$. By using

$$\frac{1}{2}\left\langle\mathsf{G}_1\cdot\mathsf{d}\boldsymbol{\rho}_0\right\rangle = \frac{J}{m\Omega}\left[\frac{1}{2}\,(\nabla\cdot\widehat{\mathsf{b}})\,\widehat{\mathsf{b}} \;+\; \nabla_\perp\ln B\right] \;+\; \frac{1}{2}\,\varrho_\|^2\,\boldsymbol{\kappa},$$

and

$$-\,\frac{1}{2}\,p_\|\;\left\langle\boldsymbol{\rho}_0\cdot\nabla\boldsymbol{\kappa}\cdot\boldsymbol{\rho}_0\right\rangle \;=\; -\,\frac{1}{2}\,J\,\varrho_\|\,(\mathbf{I}-\widehat{\mathsf{b}}\widehat{\mathsf{b}}):\nabla\boldsymbol{\kappa} \;\equiv\; -\,\frac{1}{2}\,J\,\varrho_\|\;\left(\nabla\cdot\boldsymbol{\kappa} \;+\; |\boldsymbol{\kappa}|^2\right),$$

Eq. (D 9) becomes

$$-\,\frac{1}{2}\;\left\langle\mathsf{G}_1\cdot\mathsf{d}\left[(\mathsf{G}_1\cdot\mathsf{d}\mathbf{p})\cdot\,\widehat{\mathsf{b}}\right]\right\rangle = J\,\varrho_\|\left(\boldsymbol{\kappa}\cdot\nabla\ln B - |\boldsymbol{\kappa}|^2 - \frac{1}{2}\,\nabla\cdot\boldsymbol{\kappa} - \langle\alpha_1^2\rangle\right)$$
$$+\;\frac{1}{2}\,p_\|\;\varrho_\|^2|\boldsymbol{\kappa}|^2. \tag{D 10}$$

Next, we find

$$-\,\frac{1}{2}\left\langle\boldsymbol{\rho}_0\cdot\nabla\widehat{\mathsf{b}}\cdot\;(\mathsf{G}_1\cdot\mathsf{d}\mathbf{p})\right\rangle = -\,\frac{1}{2}\left\langle C_{\rho\rho}\;\left[\boldsymbol{\rho}_0\cdot(\mathsf{G}_1\cdot\mathsf{d}\mathbf{p})\right] \;+\; C_{\rho\perp}\;\left[\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot(\mathsf{G}_1\cdot\mathsf{d}\mathbf{p})\right]\right\rangle$$
$$= \left\langle J\,\left(G_1^\theta \;+\; \boldsymbol{\rho}_0\cdot\mathbf{R}\right)\,C_{\rho\rho} \;-\; \frac{1}{2}\left(G_1^J \;-\; J\,\boldsymbol{\rho}_0\cdot\nabla\ln B\right)\,C_{\rho\perp}\right\rangle$$
$$+\;J\,\varrho_\|\left(\langle C_{\rho\rho}^2\rangle \;+\; \langle C_{\rho\perp}^2\rangle\right)$$
$$= J\,\varrho_\|\left(\langle\alpha_1^2\rangle + \frac{1}{4}\,(\nabla\cdot\widehat{\mathsf{b}})^2\right). \tag{D 11}$$

If we now combine Eqs (D 2)-(D 3), (D 5), (D 7), and (D 10)-(D 11) into Eq. (D 1), we obtain

$$m\,\frac{\partial}{\partial p_\|}\left(\frac{p_\|}{m}\,\Pi_{2\|} - \Psi_2\right) \;=\; 2\,p_\|\;\varrho_\|^2\,|\boldsymbol{\kappa}|^2 \;-\; 2\,\varrho_\|\;\widehat{\mathsf{b}}\times\boldsymbol{\kappa}\cdot\boldsymbol{\Pi}_1 \;-\; J\,\varrho_\|\;\beta_{2\|}, \tag{D 12}$$

where

$$\beta_{2\|} \;\equiv\; -\,3\,\boldsymbol{\kappa}\cdot\,(\nabla\ln B \;-\; \boldsymbol{\kappa}) \;-\; \frac{1}{4}\left[\tau^2 \;+\; (\nabla\cdot\widehat{\mathsf{b}})^2\right] \;+\; \frac{1}{2}\,\nabla\cdot\,\left[\boldsymbol{\kappa} \;+\; \widehat{\mathsf{b}}\,(\nabla\cdot\widehat{\mathsf{b}})\right].$$

Appendix E. Comparison with Previous Higher-order Guiding-center Theories

In this Appendix, we compare our results with previous higher-order guiding-center theories derived by Burby, Squire and Qin (Burby *et al.* 2013) and Parra and Calvo ((Parra & Calvo 2011) & (Parra *et al.* 2014)). In both cases, the polarization term $\boldsymbol{\Pi}_{1\perp}$ is ignored and, consequently, these theories are incomplete as discussed in Sec. 10.

For the purpose of comparison, we summarize our results here for the second-order guiding-center Hamiltonian

$$\Psi_{2(\mathrm{BT})} \;=\; \frac{1}{2}\,J\,\Omega\left(\frac{J}{m\Omega}\,\beta_{2\perp}^{(\mathrm{BT})} \;+\; \varrho_{\|}^{2}\,\beta_{2\|}^{(\mathrm{BT})}\right) \;-\; \frac{p_{\|}^{2}}{2m}\,\varrho_{\|}^{2}|\boldsymbol{\kappa}|^{2} \;+\; \boldsymbol{\Pi}_{1}\cdot\mathbf{v}_{\mathrm{gc}}, \tag{E 1}$$

where

$$\beta_{2\perp}^{(\mathrm{BT})} = -\frac{1}{2}\,\tau^{2} - \widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} + \langle\alpha_{1}^{2}\rangle + \frac{1}{2}\widehat{\mathsf{b}}\cdot\nabla\times\left(\widehat{\mathsf{b}}\times\nabla\ln B\right) - \left|\widehat{\mathsf{b}}\times\nabla\ln B\right|^{2}, \tag{E 2}$$

$$\beta_{2\|}^{(\mathrm{BT})} = -\,2\langle\alpha_{1}^{2}\rangle \;-\; 3\,\boldsymbol{\kappa}\cdot\left(\nabla\ln B \;-\; \boldsymbol{\kappa}\right) \;+\; \nabla\cdot\boldsymbol{\kappa}. \tag{E 3}$$

By using the identities (A 16)-(A 18), we obtain the following explicit expressions for the Brizard-Tronko coefficients (E 2)-(E 3):

$$\beta_{2\perp}^{(\mathrm{BT})} = \frac{1}{2}\widehat{\mathsf{b}}\cdot\nabla\times\left(\widehat{\mathsf{b}}\times\nabla\ln B\right) - \left|\widehat{\mathsf{b}}\times\nabla\ln B\right|^{2} - \frac{1}{4}\,\nabla\cdot\left[\boldsymbol{\kappa} \;-\; \widehat{\mathsf{b}}\,\left(\nabla\cdot\widehat{\mathsf{b}}\right)\right] + \frac{1}{8}\left[\left(\nabla\cdot\widehat{\mathsf{b}}\right)^{2} \;-\; 3\,\tau^{2}\right], \tag{E 4}$$

$$\beta_{2\|}^{(\mathrm{BT})} = -\,3\,\boldsymbol{\kappa}\cdot\left(\nabla\ln B \;-\; \boldsymbol{\kappa}\right) + \frac{1}{2}\,\nabla\cdot\left[\boldsymbol{\kappa} \;+\; \widehat{\mathsf{b}}\,(\nabla\cdot\widehat{\mathsf{b}})\right] - \frac{1}{4}\left[\left(\nabla\cdot\widehat{\mathsf{b}}\right)^{2} \;+\; \tau^{2}\right]. \tag{E 5}$$

We will now compare these coefficients with those obtained by Burby, Squire, and Qin (Burby *et al.* 2013) and Parra and Calvo ((Parra & Calvo 2011), (Parra *et al.* 2014)). We note, however, that these previous results assume that $\boldsymbol{\Pi}_{1} \equiv -\,\frac{1}{2}\,J\,\tau\,\widehat{\mathsf{b}}$ (i.e., $\boldsymbol{\Pi}_{1\perp} \equiv 0$) and, thus, these guiding-center theories are incomplete since they fail to yield an accurate guiding-center representation of the particle toroidal canonical momentum.

E.1. *Burby, Squire, and Qin results*

The second-order guiding-center Hamiltonian derived by Burby, Squire, and Qin (Burby *et al.* 2013) is expressed as

$$\Psi_{2(\mathrm{BSQ})} \;\equiv\; \frac{1}{2}\,J\,\Omega\left(\frac{J}{m\Omega}\,\beta_{2\perp}^{(\mathrm{BSQ})} \;+\; \varrho_{\|}^{2}\,\beta_{2\|}^{(\mathrm{BSQ})}\right) \;-\; \frac{p_{\|}^{2}}{2m}\,\varrho_{\|}^{2}|\boldsymbol{\kappa}|^{2}, \tag{E 6}$$

with the second-order coefficients

$$\beta_{2\perp}^{(\mathrm{BSQ})} = \frac{1}{2}\left[|\widehat{\mathsf{b}}\times\nabla\ln B|^{2} \;+\; \widehat{\mathsf{b}}\cdot\nabla\times\left(\widehat{\mathsf{b}}\times\nabla\ln B\right) \;-\; 3\left(|\widehat{\mathsf{b}}\times\nabla\ln B|^{2} \;+\; \left(\nabla\cdot\widehat{\mathsf{b}}\right)^{2}\right)\right] + \frac{1}{8}\left[\nabla\widehat{\mathsf{b}}:\nabla\widehat{\mathsf{b}} \;-\; 3\,\nabla\widehat{\mathsf{b}}:\left(\nabla\widehat{\mathsf{b}}\right)^{\top} \;+\; 3\,|\boldsymbol{\kappa}|^{2} \;+\; 15\,\left(\nabla\cdot\widehat{\mathsf{b}}\right)^{2}\right], \tag{E 7}$$

$$\beta_{2\|}^{(\mathrm{BSQ})} = \frac{1}{4}\left[3\,\nabla\widehat{\mathsf{b}}:\nabla\widehat{\mathsf{b}} \;-\; \nabla\widehat{\mathsf{b}}:(\nabla\widehat{\mathsf{b}})^{\top} \;+\; \left(\nabla\cdot\widehat{\mathsf{b}}\right)^{2} \;+\; |\boldsymbol{\kappa}|^{2}\right] - 3\,\boldsymbol{\kappa}\cdot\left(\nabla\ln B \;-\; \boldsymbol{\kappa}\right) \;+\; \widehat{\mathsf{b}}\cdot\nabla\left(\nabla\cdot\widehat{\mathsf{b}}\right). \tag{E 8}$$

By using the identities (A 14)-(A 15), we readily find

$$\left.\begin{array}{rcl}\beta_{2\perp}^{(\mathrm{BSQ})} & = & \beta_{2\perp}^{(\mathrm{BT})} \\ \beta_{2\|}^{(\mathrm{BSQ})} & = & \beta_{2\|}^{(\mathrm{BT})}\end{array}\right\}. \tag{E 9}$$

Since the Burby-Squire-Qin second-order guiding-center Hamiltonian is exactly equal to ours, it can be concluded that its derivation is based on an identical set of guiding-center coordinates.

E.2. *Parra-Calvo results*

The second-order guiding-center Hamiltonian derived by Parra and Calvo ((Parra & Calvo 2011), (Parra *et al.* 2014)) is expressed as

$$\Psi_{2(\mathrm{PC})} \;\equiv\; \frac{1}{2}\,J\,\Omega\left(\frac{J}{m\Omega}\,\beta_{2\perp}^{(\mathrm{PC})} \;+\; \varrho_{\|}^{2}\,\beta_{2\|}^{(\mathrm{PC})}\right) \;-\; \frac{p_{\|}^{2}}{2m}\,\varrho_{\|}^{2}|\boldsymbol{\kappa}|^{2}, \tag{E 10}$$

with the second-order coefficients

$$\begin{aligned}\beta_{2\perp}^{(\mathrm{PC})} &= \frac{1}{2B}(\mathbf{I}-\widehat{\mathsf{b}}\widehat{\mathsf{b}}):\nabla\nabla\mathbf{B}\cdot\widehat{\mathsf{b}} \;-\; \frac{3}{2B^{2}}|\nabla_{\perp}B|^{2} \;+\; \frac{1}{4}\nabla_{\perp}\widehat{\mathsf{b}}:(\nabla_{\perp}\widehat{\mathsf{b}})^{\top}\\ &\quad-\frac{1}{8}\left[(\nabla\cdot\widehat{\mathsf{b}})^{2} \;+\; \tau^{2}\right],\end{aligned} \tag{E 11}$$

$$\begin{aligned}\beta_{2\|}^{(\mathrm{PC})} &= -\,3\boldsymbol{\kappa}\cdot(\nabla\ln B-\boldsymbol{\kappa}) \;+\; \left(\nabla\widehat{\mathsf{b}}:\nabla\widehat{\mathsf{b}}-\frac{1}{2}\nabla_{\perp}\widehat{\mathsf{b}}:(\nabla_{\perp}\widehat{\mathsf{b}})^{\top}\right)\\ &\quad-\frac{1}{4}\left[3\,(\nabla\cdot\widehat{\mathsf{b}})^{2} \;-\; \tau^{2}\right].\end{aligned} \tag{E 12}$$

In order to compare the Parra-Calvo second-order Hamiltonian (E 10) with our second-order Hamiltonian, we will need the identities (A 14)-(A 15) and the following identities

$$\begin{aligned}B^{-1}(\mathbf{I}-\widehat{\mathsf{b}}\widehat{\mathsf{b}}):\nabla\nabla\mathbf{B}\cdot\widehat{\mathsf{b}} = |\widehat{\mathsf{b}}\times\nabla\ln B|^{2} \;+\; \widehat{\mathsf{b}}\cdot\nabla\times\left(\widehat{\mathsf{b}}\times\nabla\ln B\right) \;-\; \left(\nabla\cdot\widehat{\mathsf{b}}\right)^{2}\\ -\;\nabla\widehat{\mathsf{b}}:(\nabla\widehat{\mathsf{b}})^{\top} \;+\; |\boldsymbol{\kappa}|^{2},\end{aligned}$$

and

$$\nabla_{\perp}\widehat{\mathsf{b}}:(\nabla_{\perp}\widehat{\mathsf{b}})^{\top} \;=\; \nabla\widehat{\mathsf{b}}:(\nabla\widehat{\mathsf{b}})^{\top} \;-\; |\boldsymbol{\kappa}|^{2} \;=\; \nabla\widehat{\mathsf{b}}:(\nabla\widehat{\mathsf{b}}) \;+\; \tau^{2}.$$

By using these identities, we obtain the following explicit expressions for the Parra-Calvo coefficients (E 11)-(E 12):

$$\begin{aligned}\beta_{2\perp}^{(\mathrm{PC})} &= \frac{1}{2}\widehat{\mathsf{b}}\cdot\nabla\times\left(\widehat{\mathsf{b}}\times\nabla\ln B\right)-\left|\widehat{\mathsf{b}}\times\nabla\ln B\right|^{2}-\frac{1}{4}\,\nabla\cdot\left[\boldsymbol{\kappa}\;-\;\widehat{\mathsf{b}}\,\left(\nabla\cdot\widehat{\mathsf{b}}\right)\right]\\ &\quad-\frac{1}{8}\left[7\,\left(\nabla\cdot\widehat{\mathsf{b}}\right)^{2} \;+\; 3\,\tau^{2}\right],\end{aligned} \tag{E 13}$$

$$\beta_{2\|}^{(\mathrm{PC})} = -\,3\,\boldsymbol{\kappa}\cdot\left(\nabla\ln B\;-\;\boldsymbol{\kappa}\right)+\frac{1}{2}\nabla\cdot\left[\boldsymbol{\kappa}\;-\;\widehat{\mathsf{b}}\,(\nabla\cdot\widehat{\mathsf{b}})\right]-\frac{1}{4}\left[\left(\nabla\cdot\widehat{\mathsf{b}}\right)^{2} \;+\; \tau^{2}\right] \tag{E 14}$$

By comparing Eqs. (E 13)-(E 14) with Eqs. (E 4)-(E 5), we obtain the differences

$$\beta_{2\perp}^{(\mathrm{BT})}-\beta_{2\perp}^{(\mathrm{PC})} = \left(\nabla\cdot\widehat{\mathsf{b}}\right)^{2}, \tag{E 15}$$

$$\beta_{2\|}^{(\mathrm{BT})}-\beta_{2\|}^{(\mathrm{PC})} = \nabla\cdot\left[\widehat{\mathsf{b}}\,\left(\nabla\cdot\widehat{\mathsf{b}}\right)\right] \;=\; \left(\nabla\cdot\widehat{\mathsf{b}}\right)^{2} \;+\; \widehat{\mathsf{b}}\cdot\nabla\left(\nabla\cdot\widehat{\mathsf{b}}\right). \tag{E 16}$$

In more recent work, Parra and Calvo (Parra *et al.* 2014) showed that the second-order Hamiltonian difference

$$\begin{aligned}\Psi_{2(\mathrm{PC})}-\Psi_{2(\mathrm{BSQ})} &= -\,\frac{J^{2}}{2m}\left(\nabla\cdot\widehat{\mathsf{b}}\right)^{2}-\frac{1}{2}\,J\Omega\varrho_{\|}^{2}\,\nabla\cdot\left[\widehat{\mathsf{b}}\,\left(\nabla\cdot\widehat{\mathsf{b}}\right)\right]\\ &= -\,\frac{d_{0}}{dt}\left[\frac{J}{2}\,\varrho_{\|}\,\left(\nabla\cdot\widehat{\mathsf{b}}\right)\right]\equiv-\,\frac{d_{0}\langle\sigma_{3}\rangle}{dt},\end{aligned} \tag{E 17}$$

could be explained, using our notation, by adding the gyroangle-independent gauge function

$$\langle\sigma_3\rangle \;\equiv\; \frac{1}{2}\,J\,\varrho_\parallel\,(\nabla\cdot\widehat{\mathsf{b}}) \;=\; \frac{d_0}{dt}\left(\frac{J}{2\,\Omega}\right) \tag{E 18}$$

in Eq. (6.22). Hence, according to Eq. (6.2), this new gauge term introduces the following change in $G_{2\parallel}^{\mathbf{x}}$, according to Eq. (6.11):

$$G_{2\parallel}^{\mathbf{x}} \;\rightarrow\; \overline{G}_{2\parallel}^{\mathbf{x}} \;\equiv\; G_{2\parallel}^{\mathbf{x}} \;-\; \frac{\partial\langle\sigma_3\rangle}{\partial p_\parallel} \;=\; G_{2\parallel}^{\mathbf{x}} \;-\; \frac{J}{2\,m\Omega}\,\left(\nabla\cdot\widehat{\mathsf{b}}\right), \tag{E 19}$$

so that Eq. (6.23) yields the change

$$\overline{G}_2^{\mathbf{x}} \;\equiv\; G_2^{\mathbf{x}} \;-\; \frac{J\,(\nabla\cdot\widehat{\mathsf{b}})}{2m\,\Omega}\,\widehat{\mathsf{b}}, \tag{E 20}$$

and, thus, the new first-order gyroradius is now given as

$$\overline{\boldsymbol{\rho}}_1 \;\equiv\; \boldsymbol{\rho}_1 \;+\; \frac{J\,(\nabla\cdot\widehat{\mathsf{b}})}{2m\,\Omega}\,\widehat{\mathsf{b}}. \tag{E 21}$$

We note that, according to Eq. (10.3), we now find $\widehat{\mathsf{b}}\cdot\langle\overline{\boldsymbol{\rho}}_1\rangle \equiv 0$.

Lastly, the gyroangle-independent gauge function (E 18) also yields the following change in $G_2^{p_\parallel}$, according to Eq. (6.26):

$$G_2^{p_\parallel} \;\rightarrow\; \overline{G}_2^{p_\parallel} \;\equiv\; G_2^{p_\parallel} \;+\; \widehat{\mathsf{b}}\cdot\nabla\langle\sigma_3\rangle \;=\; G_2^{p_\parallel} \;+\; \frac{1}{2}\,J\,\varrho_\parallel\,\nabla\cdot\left[\widehat{\mathsf{b}}\,\left(\nabla\cdot\widehat{\mathsf{b}}\right)\right], \tag{E 22}$$

while G_1^J is unchanged, according to Eq. (6.2), because $\partial\langle\sigma_3\rangle/\partial\theta \equiv 0$. With $\overline{\Psi}_2 \equiv \Psi_{2(\mathrm{PC})}$, we immediately note that G_2^J remains unchanged according to Eq. (6.29), and that the Jacobian constraint (8.8) is still satisfied since

$$\frac{1}{B}\,\nabla\cdot\left(\langle\overline{G}_2^{\mathbf{x}}\rangle\,B\right) \;+\; \frac{\partial\overline{G}_2^{p_\parallel}}{\partial p_\parallel} \;=\; \frac{1}{B}\,\nabla\cdot\left(\langle G_2^{\mathbf{x}}\rangle\,B\right) \;+\; \frac{\partial G_2^{p_\parallel}}{\partial p_\parallel}.$$

Hence, by extending the class of Lie-transform perturbation theories with the inclusion of gyroangle-independent gauge functions (i.e., $\langle\sigma_n\rangle \neq 0$) in Sec. 3, we introduce an additional degree of freedom in the equivalence between guiding-center Hamiltonian theories.

Appendix F. Physical Interpretation of Ψ_2

In this Appendix, we provide a physical interpretation of the second-order guiding-center Hamiltonian Ψ_2. We begin with the definition of the guiding-center Hamiltonian through the guiding-center push-forward

$$H_{\mathrm{gc}} \;\equiv\; \mathsf{T}_{\mathrm{gc}}^{-1}\left(\frac{|\mathbf{p}|^2}{2m}\right) \;=\; \frac{|\mathsf{T}_{\mathrm{gc}}^{-1}\mathbf{p}|^2}{2\,m} \;=\; \frac{p_\parallel^2}{2m} \;+\; J\,\Omega \;+\; \epsilon^2\,\Psi_2. \tag{F 1}$$

While the definition does not require a gyroangle average, we shall use one here in order to remove terms that will cancel out anyway. Using the identity (9.3), we therefore obtain

$$\begin{aligned} H_{\mathrm{gc}} &\equiv \frac{m}{2}\left\langle\left|\frac{d_{\mathrm{gc}}\mathbf{X}}{dt} + \frac{d_{\mathrm{gc}}\boldsymbol{\rho}_{\mathrm{gc}}}{dt}\right|^2\right\rangle \\ &= \frac{m}{2}\left(\left|\frac{d_{\mathrm{gc}}\mathbf{X}}{dt}\right|^2 + \left\langle\left|\frac{d_{\mathrm{gc}}\boldsymbol{\rho}_{\mathrm{gc}}}{dt}\right|^2\right\rangle\right) + m\,\frac{d_{\mathrm{gc}}\mathbf{X}}{dt}\cdot\left\langle\frac{d_{\mathrm{gc}}\boldsymbol{\rho}_{\mathrm{gc}}}{dt}\right\rangle. \end{aligned} \tag{F 2}$$

where the guiding-center kinetic energy

$$\frac{m}{2}\left|\frac{d_{\rm gc}\mathbf{X}}{dt}\right|^2 \;=\; \frac{p_{\|}^2}{2m} \;+\; \epsilon^2\left(\frac{m}{2}\,|\mathbf{v}_{\rm gc}|^2 \;+\; p_{\|}\,\frac{\partial\Psi_2}{\partial p_{\|}}\right) \tag{F 3}$$

includes the second-order guiding-center kinetic energy associated with the guiding-center drift velocity and the term $p_{\|}\,\partial\Psi_2/\partial p_{\|}$, while

$$m\,\frac{d_{\rm gc}\mathbf{X}}{dt}\boldsymbol{\cdot}\left\langle\frac{d_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{dt}\right\rangle \;=\; \epsilon^2\,p_{\|}\,\widehat{\mathsf{b}}\boldsymbol{\cdot}\frac{d_0\langle\boldsymbol{\rho}_1\rangle}{dt}.$$

Lastly, the "gyration" kinetic energy is

$$\begin{aligned}\frac{m}{2}\left\langle\left|\frac{d_{\rm gc}\boldsymbol{\rho}_{\rm gc}}{dt}\right|^2\right\rangle = J\,\Omega \;&+\; \epsilon\,\left\langle\mathbf{p}_\perp\boldsymbol{\cdot}\left(\Omega\,\frac{\partial\boldsymbol{\rho}_1}{\partial\theta} \;+\; \frac{d_0\boldsymbol{\rho}_0}{dt}\right)\right\rangle\\ &+\epsilon^2\left\langle\mathbf{p}_\perp\boldsymbol{\cdot}\left(\Omega\,\frac{\partial\boldsymbol{\rho}_2}{\partial\theta} \;+\; \frac{\partial\Psi_2}{\partial J}\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} \;+\; \frac{d_0\boldsymbol{\rho}_1}{dt} \;+\; \frac{d_1\boldsymbol{\rho}_0}{dt}\right)\right\rangle\\ &+\epsilon^2\,\frac{m}{2}\,\left\langle\left|\Omega\,\frac{\partial\boldsymbol{\rho}_1}{\partial\theta} \;+\; \frac{d_0\boldsymbol{\rho}_0}{dt}\right|^2\right\rangle,\end{aligned} \tag{F 4}$$

where

$$\left\langle\mathbf{p}_\perp\boldsymbol{\cdot}\left(\frac{\partial\Psi_2}{\partial J}\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right)\right\rangle \;=\; 2\,J\,\frac{\partial\Psi_2}{\partial J},$$

and

$$\begin{aligned}\Omega\,\frac{\partial\boldsymbol{\rho}_1}{\partial\theta} \;+\; \frac{d_0\boldsymbol{\rho}_0}{dt} = \frac{p_{\|}}{m}&\left[(\boldsymbol{\rho}_0\boldsymbol{\cdot}\boldsymbol{\kappa})\,\widehat{\mathsf{b}} \;+\; \left(\frac{1}{2}\,\nabla\boldsymbol{\cdot}\widehat{\mathsf{b}} \;-\; \alpha_2\right)\boldsymbol{\rho}_0 \;-\; \frac{1}{2}\,\alpha_1\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right]\\ &+\frac{J}{m}\left(\alpha_1\,\widehat{\mathsf{b}} \;-\; 2\,\mathsf{a}_1\boldsymbol{\cdot}\nabla\ln B\right),\end{aligned} \tag{F 5}$$

Here, it is a simple task to show that the first-order terms vanish

$$\left\langle\mathbf{p}_\perp\boldsymbol{\cdot}\left(\Omega\,\frac{\partial\boldsymbol{\rho}_1}{\partial\theta} \;+\; \frac{d_0\boldsymbol{\rho}_0}{dt}\right)\right\rangle \;=\; -\,J\,\Omega\left(\varrho_{\|}\,\langle\alpha_1\rangle\right) \;=\; 0.$$

Hence, we see that the higher-order terms associated with magnetic nonuniformity enter at the second order.

By combining the remaining components, we now obtain the second-order equation

$$\begin{aligned}\Psi_2 \equiv \frac{m}{2}\,|\mathbf{v}_{\rm gc}|^2 \;&+\; \left(p_{\|}\,\frac{\partial\Psi_2}{\partial p_{\|}} \;+\; 2\,J\,\frac{\partial\Psi_2}{\partial J}\right)\\ &+\;\left[\Psi_{2(A)} \;+\; \Psi_{2(B)} \;+\; \Psi_{2(C)} \;+\; \Psi_{2(D)} \;+\; \Psi_{2(E)}\right],\end{aligned} \tag{F 6}$$

where we defined

$$\Psi_{2(A)} \equiv \frac{m}{2} \left\langle \left| \Omega \frac{\partial \boldsymbol{\rho}_1}{\partial \theta} + \frac{d_0 \boldsymbol{\rho}_0}{dt} \right|^2 \right\rangle, \tag{F 7}$$

$$\Psi_{2(B)} \equiv p_{\|} \, \widehat{\mathsf{b}} \cdot \frac{d_0 \langle \boldsymbol{\rho}_1 \rangle}{dt}, \tag{F 8}$$

$$\Psi_{2(C)} \equiv \left\langle \mathbf{p}_{\perp} \cdot \frac{d_1 \boldsymbol{\rho}_0}{dt} \right\rangle, \tag{F 9}$$

$$\Psi_{2(D)} \equiv \left\langle \mathbf{p}_{\perp} \cdot \frac{d_0 \boldsymbol{\rho}_1}{dt} \right\rangle, \tag{F 10}$$

$$\Psi_{2(E)} \equiv \left\langle \mathbf{p}_{\perp} \cdot \left(\Omega \frac{\partial \boldsymbol{\rho}_2}{\partial \theta} \right) \right\rangle. \tag{F 11}$$

First, using Eq. (F 5), we find

$$\Psi_{2(A)} = \frac{J^2}{2m} \left(\langle \alpha_1^2 \rangle + |\nabla_{\perp} \ln B|^2 \right) + \frac{1}{2} J\Omega \, \varrho_{\|}^2 \left[|\boldsymbol{\kappa}|^2 + \langle \alpha_1^2 \rangle + \frac{1}{2} (\nabla \cdot \widehat{\mathsf{b}})^2 \right]. \tag{F 12}$$

Second, using Eq. (10.3), we find

$$\begin{aligned} \Psi_{2(B)} &= \frac{p_{\|}^2}{m} \left[\widehat{\mathsf{b}} \cdot \nabla \left(\langle \boldsymbol{\rho}_1 \rangle \cdot \widehat{\mathsf{b}} \right) - \boldsymbol{\kappa} \cdot \langle \boldsymbol{\rho}_1 \rangle \right] \\ &= -\frac{1}{2} J\Omega \, \varrho_{\|}^2 \left\{ \nabla \cdot \left[\widehat{\mathsf{b}} \left(\nabla \cdot \widehat{\mathsf{b}} \right) \right] - 3 \, \boldsymbol{\kappa} \cdot \nabla \ln B \right\} + \frac{p_{\|}^2}{m} \, \varrho_{\|}^2 |\boldsymbol{\kappa}|^2 \\ &\quad - \boldsymbol{\Pi}_1 \cdot \frac{\widehat{\mathsf{b}}}{m} \times \left(\frac{p_{\|}^2}{m\Omega} \, \boldsymbol{\kappa} \right). \end{aligned} \tag{F 13}$$

Third, using

$$\begin{aligned} \frac{d_1 \boldsymbol{\rho}_0}{dt} &\equiv \mathbf{v}_{\rm gc} \cdot \nabla_0^* \boldsymbol{\rho}_0 = -J \, \mathbf{v}_{\rm gc} \cdot \nabla \ln B \, \frac{\partial \rho_0}{\partial J} + \frac{1}{2} \, \mathbf{v}_{\rm gc} \cdot \nabla \times \widehat{\mathsf{b}} \, \frac{\partial \rho_0}{\partial \theta} \\ &\quad - \mathbf{v}_{\rm gc} \cdot \left(C_{\perp \rho} \frac{\partial \rho_0}{\partial \theta} + C_{\rho\rho} \, \boldsymbol{\rho}_0 \right) \widehat{\mathsf{b}}, \end{aligned}$$

we find

$$\Psi_{2(C)} = \left(\frac{1}{2} \, \mathbf{v}_{\rm gc} \cdot \nabla \times \widehat{\mathsf{b}} \right) \left\langle \frac{\partial \boldsymbol{\rho}_0}{\partial \theta} \cdot \mathbf{p}_{\perp} \right\rangle = \left(J \, \nabla \times \widehat{\mathsf{b}} \right) \cdot \mathbf{v}_{\rm gc} \equiv -2 \, \boldsymbol{\Pi}_1 \cdot \mathbf{v}_{\rm gc}. \tag{F 14}$$

Hence, both Eqs. (F 13)-(F 14) contain direct contributions of the polarization term $\boldsymbol{\Pi}_{1\perp}$ to the second-order guiding-center Hamiltonian.

Fourth, we find

$$\begin{aligned} \Psi_{2(D)} &= \frac{d_0}{dt} \langle \mathbf{p}_{\perp} \cdot \boldsymbol{\rho}_1 \rangle - \left\langle \frac{d_0 \mathbf{p}_{\perp}}{dt} \cdot \boldsymbol{\rho}_1 \right\rangle = - \left\langle \frac{d_0 \mathbf{p}_{\perp}}{dt} \cdot \boldsymbol{\rho}_1 \right\rangle \\ &= -p_{\|} \Omega \left[\left\langle (\boldsymbol{\kappa} \cdot \boldsymbol{\rho}_0) \, \widehat{\mathsf{b}} \cdot \frac{\partial \boldsymbol{\rho}_1}{\partial \theta} \right\rangle - \frac{1}{2} \, \tau \left\langle \frac{\partial \boldsymbol{\rho}_0}{\partial \theta} \cdot \frac{\partial \boldsymbol{\rho}_1}{\partial \theta} \right\rangle \right], \end{aligned}$$

where we used

$$\langle \mathbf{p}_{\perp} \cdot \boldsymbol{\rho}_1 \rangle = -m\Omega \left\langle \boldsymbol{\rho}_0 \cdot \frac{\partial \boldsymbol{\rho}_1}{\partial \theta} \right\rangle = 2 \, J \, \varrho_{\|} \, \langle \alpha_2 \rangle \equiv 0,$$

and

$$\frac{d_0\mathbf{p}_\perp}{dt} \;\equiv\; \frac{p_\|}{m}\widehat{\mathsf{b}}\cdot\nabla_0^*\mathbf{p}_\perp \;=\; -\,\frac{p_\|}{m}\left[\frac{1}{2}\left(\nabla\cdot\widehat{\mathsf{b}}\right)\mathbf{p}_\perp \;-\; \frac{1}{2}\,\tau\,\frac{\partial\mathbf{p}_\perp}{\partial\theta} \;+\; \left(\mathbf{p}_\perp\cdot\boldsymbol{\kappa}\right)\widehat{\mathsf{b}}\right].$$

Here,

$$-\,p_\|\,\Omega\,\left\langle\left(\boldsymbol{\kappa}\cdot\boldsymbol{\rho}_0\right)\,\widehat{\mathsf{b}}\cdot\frac{\partial\boldsymbol{\rho}_1}{\partial\theta}\right\rangle \;=\; -\,2\,J\,\Omega\,\varrho_\|^2\,|\boldsymbol{\kappa}|^2$$

and

$$\frac{1}{2}\,p_\|\,\Omega\,\tau\,\left\langle\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\frac{\partial\boldsymbol{\rho}_1}{\partial\theta}\right\rangle \;=\; -\,\frac{1}{2}\,J\,\Omega\,\varrho_\|^2\,\tau^2.$$

Hence, we find

$$\Psi_{2(D)} \;=\; -\,J\Omega\,\varrho_\|^2\left(2\,|\boldsymbol{\kappa}|^2 \;+\; \frac{1}{2}\,\tau^2\right). \tag{F 15}$$

Lastly, we write

$$\Psi_{2(E)} = m\Omega^2\,\langle\boldsymbol{\rho}_0\cdot\boldsymbol{\rho}_2\rangle \;\equiv\; \Psi_{2(E)}^{(1)} + \Psi_{2(E)}^{(2)} + \Psi_{2(E)}^{(3)}, \tag{F 16}$$

where

$$\begin{aligned}\Psi_{2(E)}^{(1)} \;\equiv\; -\,m\Omega^2\langle\boldsymbol{\rho}_0\cdot G_3^{\mathbf{x}}\rangle &= -\,p_\|\Omega\left\langle\left(\boldsymbol{\kappa}\cdot\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right)\,G_{2\|}^{\mathbf{x}} - \tau\,\left(\boldsymbol{\rho}_0\cdot G_2^{\mathbf{x}}\right)\right\rangle \\ &\quad +\;\left\langle\Omega\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\left[D_1^2(\mathbf{P}_3) + \nabla\sigma_3\right]\right\rangle,\end{aligned} \tag{F 17}$$

which makes use of $G_3^{\mathbf{X}}$,

$$\begin{aligned}\Psi_{2(E)}^{(2)} \equiv -\,m\Omega^2\left\langle\boldsymbol{\rho}_0\cdot\left(\mathsf{G}_2\cdot\,\mathsf{d}\boldsymbol{\rho}_0\right)\right\rangle \;&=\; -\,\frac{m\Omega^2}{2}\,\left\langle\mathsf{G}_2\cdot\mathsf{d}\left(\frac{2\,J}{m\Omega}\right)\right\rangle \\ = -\,\Omega\,\langle G_2^J\rangle \;+\; J\,\Omega\,\langle G_2^{\mathbf{x}}\rangle\cdot\nabla\ln B,&\end{aligned} \tag{F 18}$$

which makes use of the components of G_2, and

$$\begin{aligned}\Psi_{2(E)}^{(3)} &\equiv \frac{1}{6}\,m\Omega^2\left\langle\boldsymbol{\rho}_0\cdot\left[\mathsf{G}_1\cdot\,\mathsf{d}\left(\mathsf{G}_1\cdot\mathsf{d}\boldsymbol{\rho}_0\right)\right]\right\rangle \\ &= \frac{1}{6}\,B\Omega\left\langle\mathsf{G}_1\cdot\mathsf{d}\left[B^{-1}\,\left(G_1^J \;+\; J\,\boldsymbol{\rho}_0\cdot\nabla\ln B\right)\right]\right\rangle \;-\; \frac{1}{6}\,m\,\Omega^2\left\langle\left|\mathsf{G}_1\cdot\mathsf{d}\boldsymbol{\rho}_0\right|^2\right\rangle.\end{aligned} \tag{F 19}$$

In Eq. (F 17), we find

$$-\,p_\|\Omega\left\langle\left(\boldsymbol{\kappa}\cdot\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right)\,G_{2\|}^{\mathbf{x}} - \tau\,\left(\boldsymbol{\rho}_0\cdot G_2^{\mathbf{x}}\right)\right\rangle \;=\; -\,J\,\Omega\,\varrho_\|^2\left(2\,|\boldsymbol{\kappa}|^2 \;-\; \frac{3}{2}\,\tau^2\right). \tag{F 20}$$

Using Eq. (6.22), we also find

$$\begin{aligned}\left\langle\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\nabla\sigma_3\right\rangle &= \nabla\cdot\left\langle\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\,\sigma_3\right\rangle \;-\; \left\langle\sigma_3\,\left(\nabla\cdot\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right)\right\rangle \\ &= -\,\frac{1}{3}\,p_\|\left[\nabla\cdot\left\langle\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\,G_{2\|}^{\mathbf{x}}\right\rangle \;-\; \left\langle G_{2\|}^{\mathbf{x}}\,\left(\nabla\cdot\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right)\right\rangle\right] \\ &= -\,\frac{2}{3}\,J\,\varrho_\|^2\left[B^2\,\nabla\cdot\left(\frac{\boldsymbol{\kappa}}{B^2}\right) \;+\; \boldsymbol{\kappa}\cdot\left(\frac{1}{2}\,\nabla\ln B \;+\; \boldsymbol{\kappa} \;+\; \widehat{\mathsf{b}}\times\mathbf{R}\right)\right].\end{aligned} \tag{F 21}$$

Next, we need

$$\left\langle \frac{\partial \boldsymbol{\rho}_0}{\partial \theta} \cdot D_1^2(\mathbf{P}_3) \right\rangle = \frac{2J}{m\Omega}\, \widehat{\mathsf{b}} \cdot \nabla \times \langle D_1(\mathbf{P}_3) \rangle \;+\; \left\langle G_1^{p_\parallel}\, \frac{\partial}{\partial p_\parallel} \left(D_1(\mathbf{P}_3) \cdot \frac{\partial \boldsymbol{\rho}_0}{\partial \theta} \right) \right\rangle$$
$$+\; \left\langle G_1^J \left[\frac{\partial}{\partial J} \left(D_1(\mathbf{P}_3) \cdot \frac{\partial \boldsymbol{\rho}_0}{\partial \theta} \right) \;-\; D_1(\mathbf{P}_3) \cdot \frac{\partial^2 \boldsymbol{\rho}_0}{\partial J \partial \theta} \right] \right\rangle$$
$$+\; \left\langle G_1^\theta \left[\frac{\partial}{\partial \theta} \left(D_1(\mathbf{P}_3) \cdot \frac{\partial \boldsymbol{\rho}_0}{\partial \theta} \right) \;+\; D_1(\mathbf{P}_3) \cdot \boldsymbol{\rho}_0 \right] \right\rangle,$$

where

$$\langle D_1(\mathbf{P}_3) \rangle = \frac{1}{3}\, J \left(2\,\mathbf{R} \;+\; \frac{1}{2}\,\tau\, \widehat{\mathsf{b}} \right) \;-\; \frac{\widehat{\mathsf{b}}}{3} \times \left(J\, \nabla \ln B \;+\; \frac{p_\parallel^2}{m\Omega}\, \boldsymbol{\kappa} \right),$$
$$D_1(\mathbf{P}_3) \cdot \frac{\partial \boldsymbol{\rho}_0}{\partial \theta} = \frac{1}{3}\, J\, \varrho_\parallel (2\,\tau - \alpha_1) \;+\; \frac{1}{3}\, \boldsymbol{\rho}_0 \cdot \left(2\,J\, \widehat{\mathsf{b}} \times \mathbf{R} \;+\; \frac{p_\parallel^2}{m\Omega}\, \boldsymbol{\kappa} \right),$$
$$D_1(\mathbf{P}_3) \cdot \boldsymbol{\rho}_0 = \frac{1}{3}\, D_1(\mathbf{p}_\perp) \cdot \boldsymbol{\rho}_0 \;=\; -\,\frac{2}{3}\, J\, G_1^\theta.$$

First, we find

$$\frac{2J}{m\Omega}\, \widehat{\mathsf{b}} \cdot \nabla \times \langle D_1(\mathbf{P}_3) \rangle = \frac{J^2}{3\,m\Omega} \left(4\, \widehat{\mathsf{b}} \cdot \nabla \times \mathbf{R} \;+\; \tau^2 \right)$$
$$-\; \frac{2J}{3\,m\Omega}\, \widehat{\mathsf{b}} \cdot \nabla \times \left[\widehat{\mathsf{b}} \times \left(J\, \nabla \ln B \;+\; \frac{p_\parallel^2}{m\Omega}\, \boldsymbol{\kappa} \right) \right]. \qquad \text{(F 22)}$$

Next, we find

$$\left\langle G_1^{p_\parallel}\, \frac{\partial}{\partial p_\parallel} \left(D_1(\mathbf{P}_3) \cdot \frac{\partial \boldsymbol{\rho}_0}{\partial \theta} \right) \right\rangle = \left\langle G_1^{p_\parallel} \left[\frac{J}{3\,m\Omega}\, (2\tau - \alpha_1) \;+\; \frac{2}{3}\, \varrho_\parallel\, (\boldsymbol{\rho}_0 \cdot \boldsymbol{\kappa}) \right] \right\rangle$$
$$= \frac{J^2}{3\,m\Omega} \left(2\,\tau^2 \;-\; \langle \alpha_1^2 \rangle \right) \;-\; \frac{2}{3}\, J\, \varrho_\parallel^2\, |\boldsymbol{\kappa}|^2, \qquad \text{(F 23)}$$

and

$$\left\langle G_1^J \left[\frac{\partial}{\partial J} \left(D_1(\mathbf{P}_3) \cdot \frac{\partial \boldsymbol{\rho}_0}{\partial \theta} \right) - D_1(\mathbf{P}_3) \cdot \frac{\partial^2 \boldsymbol{\rho}_0}{\partial J \partial \theta} \right] \right\rangle$$
$$=\; \left\langle G_1^J \left[\frac{1}{6}\, \varrho_\parallel\, (2\tau - \alpha_1) + \frac{2}{3}\, \frac{\partial \boldsymbol{\rho}_0}{\partial \theta} \cdot \mathbf{R} \right] \right\rangle$$
$$=\; -\,\frac{1}{6}\, J\, \varrho_\parallel^2 \left(2\,\tau^2 \;-\; \langle \alpha_1^2 \rangle \right) \qquad \text{(F 24)}$$
$$+\; \frac{2\,J}{3\,m\Omega}\, \widehat{\mathsf{b}} \times \mathbf{R} \cdot \left(J\, \nabla \ln B \;+\; \frac{p_\parallel^2}{m\Omega}\, \boldsymbol{\kappa} \right)$$

and

$$\begin{aligned}
& \left\langle G_1^\theta \left[\frac{\partial}{\partial\theta} \left(D_1(\mathbf{P}_3)\cdot\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right) \;+\; D_1(\mathbf{P}_3)\cdot\boldsymbol{\rho}_0 \right] \right\rangle \\
&\quad = \frac{2}{3}\,J\,\left\langle G_1^\theta \left(\varrho_\parallel\,\alpha_2 \;-\; \frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\nabla\ln B \right) \right\rangle \\
&\quad = \frac{1}{6}\,J\,\varrho_\parallel^2\,\left(\langle\alpha_1^2\rangle \;-\; 2\,\boldsymbol{\kappa}\cdot\nabla\ln B \right) \\
&\qquad -\; \frac{2\,J^2}{3\,m\Omega}\,\nabla\ln B\cdot\left(\nabla\ln B + \widehat{\mathsf{b}}\times\mathbf{R} \right)
\end{aligned} \tag{F 25}$$

Hence, by combining Eqs. (F 20)-(F 25) into Eq. (F 17), we obtain

$$\begin{aligned}
\Psi_{2(E)}^{(1)} &= \frac{J^2}{3\,m}\left[4\,\widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} \;+\; 3\,\tau^2 \;-\; \langle\alpha_1^2\rangle \;-\; 2\,|\widehat{\mathsf{b}}\times\nabla\ln B|^2 \;-\; 2\,\widehat{\mathsf{b}}\cdot\nabla\times\left(\widehat{\mathsf{b}}\times\nabla\ln B\right) \right] \\
&\quad -\; \frac{1}{3}\,J\Omega\,\varrho_\parallel^2\left[4\,\nabla\cdot\boldsymbol{\kappa} \;-\; 4\,\boldsymbol{\kappa}\cdot\nabla\ln B \;+\; 12\,|\boldsymbol{\kappa}|^2 \;-\; \frac{7}{2}\,\tau^2 \;-\; \langle\alpha_1^2\rangle \right],
\end{aligned} \tag{F 26}$$

where the gyrogauge-dependent terms cancel out. Next, using the definition (6.31), Eq. (F 18) can be expressed as

$$\begin{aligned}
\Psi_{2(E)}^{(2)} &= \Psi_2 \;+\; \frac{m}{2}\,|\mathbf{v}_{\rm gc}|^2 \;-\; \boldsymbol{\Pi}_1\cdot\mathbf{v}_{\rm gc} - J\Omega\,\varrho_\parallel^2\left(\frac{1}{2}\,\tau^2 \;-\; \langle\alpha_1^2\rangle \right) \\
&\quad +\, J\,\Omega\,\nabla\ln B\cdot\left[-\,\boldsymbol{\Pi}_1\times\frac{\widehat{\mathsf{b}}}{m\Omega} \;+\; \frac{1}{2}\left(\frac{J}{m\Omega}\,\nabla_\perp\ln B \;+\; \varrho_\parallel^2\,\boldsymbol{\kappa} \right) \right]
\end{aligned} \tag{F 27}$$

Lastly, the two terms in Eq. (F 19) are

$$\begin{aligned}
& \frac{1}{6}\,B\Omega\left\langle \mathsf{G}_1\cdot\mathsf{d}\left[B^{-1}\,\left(G_1^J \;+\; J\,\boldsymbol{\rho}_0\cdot\nabla\ln B \right) \right] \right\rangle \\
&= \frac{\Omega}{6}\,\left\langle \left[\boldsymbol{\rho}_0\cdot\nabla\ln B \;+\; (\nabla\cdot\boldsymbol{\rho}_0) \right]\,\left(G_1^J \;+\; J\,\boldsymbol{\rho}_0\cdot\nabla\ln B \right) \right\rangle \\
&\quad -\; \frac{\Omega}{6}\,\nabla\cdot\left\langle \boldsymbol{\rho}_0\,\left(G_1^J \;+\; J\,\boldsymbol{\rho}_0\cdot\nabla\ln B \right) \right\rangle \;+\; \frac{\Omega}{6}\,\left\langle G_1^{p_\parallel}\,\frac{\partial}{\partial p_\parallel}\left(G_1^J \;+\; J\,\boldsymbol{\rho}_0\cdot\nabla\ln B \right) \right\rangle \\
&\quad +\; \frac{\Omega}{6}\,\left\langle G_1^J\,\frac{\partial}{\partial J}\left(G_1^J \;+\; J\,\boldsymbol{\rho}_0\cdot\nabla\ln B \right) \;+\; G_1^\theta\,\frac{\partial}{\partial\theta}\left(G_1^J \;+\; J\,\boldsymbol{\rho}_0\cdot\nabla\ln B \right) \right\rangle \\
&= \frac{J}{6\,m}\left(\frac{1}{2}\,\nabla\ln B - \boldsymbol{\kappa} - \widehat{\mathsf{b}}\times\mathbf{R} \right)\cdot\left(2J\,\nabla\ln B \;+\; \frac{p_\parallel^2}{m\Omega}\,\boldsymbol{\kappa} \right) \\
&\quad -\; \frac{\Omega}{6}\,\left\{ \nabla\cdot\left[\frac{J}{m\Omega}\,\left(2\,J\,\nabla_\perp\ln B \;+\; \frac{p_\parallel^2}{m\Omega}\,\boldsymbol{\kappa} \right) \right] \;+\; \frac{J^2}{m\Omega}\,\left(\tau^2 + \langle\alpha_1^2\rangle \right) \;+\; 2\,J\,\varrho_\parallel^2\,|\boldsymbol{\kappa}|^2 \right\} \\
&\quad +\; \frac{1}{6\,m}\left(J\,\nabla\ln B \;+\; \frac{p_\parallel^2}{m\Omega}\,\boldsymbol{\kappa} \right)\cdot\left(3J\,\nabla\ln B \;+\; \frac{p_\parallel^2}{2\,m\Omega}\,\boldsymbol{\kappa} \right) \;+\; \frac{1}{6}\,J\Omega\,\varrho_\parallel^2\,\left(\tau^2 \;+\; \langle\alpha_1^2\rangle \right) \\
&\quad +\; \frac{J}{6\,m}\left(\nabla\ln B \;+\; \frac{p_\parallel^2\,\boldsymbol{\kappa}}{2J\,m\Omega} \;+\; \widehat{\mathsf{b}}\times\mathbf{R} \right)\cdot\left(2J\,\nabla\ln B \;+\; \frac{p_\parallel^2}{m\Omega}\,\boldsymbol{\kappa} \right) \;+\; \frac{1}{6}\,J\,\Omega\,\varrho_\parallel^2\,\langle\alpha_1^2\rangle,
\end{aligned} \tag{F 28}$$

and

$$- \frac{1}{6}\, m\,\Omega^2 \left\langle |\mathsf{G}_1 \cdot \mathsf{d}\boldsymbol{\rho}_0|^2 \right\rangle = - \frac{J^2}{6\,m} \left\langle \left(\nabla\cdot\widehat{\mathsf{b}} - 4\,\alpha_2 \right)^2 \right\rangle - \frac{1}{3}\, J\,\Omega \left\langle \left(G_1^\theta + \boldsymbol{\rho}_0\cdot\mathbf{R} \right)^2 \right\rangle \tag{F 29}$$

$$- \frac{\Omega}{12\,J} \left\langle \left(G_1^J \;+\; J\;\boldsymbol{\rho}_0\cdot\nabla\ln B \right)^2 \right\rangle$$

$$= - \frac{J^2}{6\,m} \left[\left(\nabla\cdot\widehat{\mathsf{b}} \right)^2 + 4\,\langle\alpha_1^2\rangle \right] - \frac{1}{12\,m} \left| 2\,J\,\nabla\ln B + \frac{p_\parallel^2}{m\Omega}\,\boldsymbol{\kappa} \right|^2$$

$$- \frac{1}{12} J\Omega\, \varrho_\parallel^2 \left(\tau^2 +\; 2\,\langle\alpha_1^2\rangle \right) - \frac{J^2}{3\,m} \left| \nabla_\perp \ln B + \frac{p_\parallel^2\,\boldsymbol{\kappa}}{2J\;m\Omega} \right|^2 .$$

Hence, combining Eqs. (F 28)-(F 29) into Eq. (F 19), we obtain

$$\Psi_{2(E)}^{(3)} = \frac{J^2}{3\,m} \left[|\widehat{\mathsf{b}}\times\nabla\ln B|^2 \;-\; \boldsymbol{\kappa}\cdot\nabla\ln B \;-\; B\,\nabla\cdot\left(B^{-1}\,\nabla_\perp\ln B \right) \right.$$
$$\left. - \frac{1}{2} \left(5\,\langle\alpha_1^2\rangle \;+\; \tau^2 \;+\; (\nabla\cdot\widehat{\mathsf{b}})^2 \right) \right] \;+\; \frac{1}{3}\, J\Omega\, \varrho_\parallel^2 \left[\boldsymbol{\kappa}\cdot\nabla\ln B \right.$$
$$\left. - \frac{1}{2}\, B^2\,\nabla\cdot\left(\frac{\boldsymbol{\kappa}}{B^2} \right) \;-\; \frac{1}{2} \left(3\,|\boldsymbol{\kappa}|^2 \;-\; \frac{1}{2}\,\tau^2 \;-\; \langle\alpha_1^2\rangle \right) \right], \tag{F 30}$$

and the gyrogauge-dependent terms have once again cancelled each other.

We now combine Eqs. (F 12)-(F 15), (F 26)-(F 27), and (F 30), so that we obtain

$$\Psi_2 \equiv \frac{m}{2}\,|\mathbf{v}_{\rm gc}|^2 \;+\; p_\parallel\,\frac{\partial\Psi_2}{\partial p_\parallel} \;+\; 2\,J\,\frac{\partial\Psi_2}{\partial J} \;+\; \frac{J^2}{2m} \left(\langle\alpha_1^2\rangle \;+\; |\nabla_\perp\ln B|^2 \right)$$
$$+ \frac{1}{2}\, J\Omega\, \varrho_\parallel^2 \left[|\boldsymbol{\kappa}|^2 \;+\; \langle\alpha_1^2\rangle \;+\; \frac{1}{2}\,(\nabla\cdot\widehat{\mathsf{b}})^2 \right]$$
$$- \frac{1}{2}\, J\Omega\, \varrho_\parallel^2 \left\{ \nabla\cdot\left[\widehat{\mathsf{b}}\, \left(\nabla\cdot\widehat{\mathsf{b}} \right) \right] \;-\; 3\,\boldsymbol{\kappa}\cdot\nabla\ln B \right\} \;+\; \frac{p_\parallel^2}{m}\,\varrho_\parallel^2 |\boldsymbol{\kappa}|^2$$
$$- \boldsymbol{\Pi}_1\cdot\frac{\widehat{\mathsf{b}}}{m}\times\left(\frac{p_\parallel^2}{m\Omega}\,\boldsymbol{\kappa} \right) \;-\; 2\,\boldsymbol{\Pi}_1\cdot\mathbf{v}_{\rm gc} \;-\; J\Omega\,\varrho_\parallel^2 \left(2\,|\boldsymbol{\kappa}|^2 + \frac{1}{2}\,\tau^2 \right)$$
$$+ \frac{J^2}{3\,m} \left[4\,\widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} + 3\,\tau^2 - \langle\alpha_1^2\rangle - 2\,|\widehat{\mathsf{b}}\times\nabla\ln B|^2 - 2\,\widehat{\mathsf{b}}\cdot\nabla\times\left(\widehat{\mathsf{b}}\times\nabla\ln B \right) \right]$$
$$- \frac{1}{3}\, J\Omega\, \varrho_\parallel^2 \left[4\,\nabla\cdot\boldsymbol{\kappa} \;-\; 4\,\boldsymbol{\kappa}\cdot\nabla\ln B \;+\; 12\,|\boldsymbol{\kappa}|^2 \;-\; \frac{7}{2}\,\tau^2 \;-\; \langle\alpha_1^2\rangle \right]$$
$$+ \Psi_2 \;+\; \frac{m}{2}\,|\mathbf{v}_{\rm gc}|^2 \;-\; \boldsymbol{\Pi}_1\cdot\mathbf{v}_{\rm gc} - J\Omega\,\varrho_\parallel^2 \left(\frac{1}{2}\,\tau^2 \;-\; \langle\alpha_1^2\rangle \right)$$
$$+ J\,\Omega\,\nabla\ln B\cdot \left[-\,\boldsymbol{\Pi}_1\times\frac{\widehat{\mathsf{b}}}{m\Omega} \;+\; \frac{1}{2} \left(\frac{J}{m\Omega}\,\nabla_\perp\ln B \;+\; \varrho_\parallel^2\,\boldsymbol{\kappa} \right) \right]$$
$$+ \frac{J^2}{3\,m} \left[|\widehat{\mathsf{b}}\times\nabla\ln B|^2 \;-\; \boldsymbol{\kappa}\cdot\nabla\ln B \;-\; B\,\nabla\cdot\left(B^{-1}\,\nabla_\perp\ln B \right) \right.$$
$$\left. - \frac{1}{2} \left(5\,\langle\alpha_1^2\rangle \;+\; \tau^2 \;+\; (\nabla\cdot\widehat{\mathsf{b}})^2 \right) \right]$$
$$+ \frac{1}{3}\, J\Omega\, \varrho_\parallel^2 \left[\boldsymbol{\kappa}\cdot\nabla\ln B \;-\; \frac{1}{2}\, B^2\,\nabla\cdot\left(\frac{\boldsymbol{\kappa}}{B^2} \right) \;-\; \frac{1}{2} \left(3\,|\boldsymbol{\kappa}|^2 \;-\; \frac{1}{2}\,\tau^2 \;-\; \langle\alpha_1^2\rangle \right) \right],$$

which can be simplified to the final expression

$$
\begin{aligned}
-\,p_\| \frac{\partial\Psi_2}{\partial p_\|} - 2\,J\,\frac{\partial\Psi_2}{\partial J} = {} & 2\,\frac{p_\|^2}{m}\,\varrho_\|^2\,|\boldsymbol{\kappa}|^2 \;-\; 4\,\mathbf{\Pi}_1\cdot\mathbf{v}_{\rm gc} \\
& + \frac{J^2}{3\,m}\left[5\,|\nabla_\perp\ln B|^2 \;-\; 2\,\langle\alpha_1^2\rangle \;+\; 4\,\widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} \;-\; 2\,\widehat{\mathsf{b}}\cdot\nabla\times\left(\widehat{\mathsf{b}}\times\nabla\ln B\right)\right. \\
& \left. -\; B\,\nabla\cdot\left(\frac{\nabla_\perp\ln B}{B}\right) \;-\; \boldsymbol{\kappa}\cdot\nabla\ln B \;+\; \frac{1}{2}\left(5\,\tau^2 \;-\; (\nabla\cdot\widehat{\mathsf{b}})^2\right)\right] \\
& + \frac{1}{3}\,J\,\Omega\,\varrho_\|^2\left[17\,\boldsymbol{\kappa}\cdot\nabla\ln B \;-\; \frac{B^2}{2}\,\nabla\cdot\left(\frac{\boldsymbol{\kappa}}{B^2}\right) \;-\; 18\,|\boldsymbol{\kappa}|^2 \;-\; 4\,\nabla\cdot\boldsymbol{\kappa}\right. \\
& \left. +\; \frac{3}{4}\left(\tau^2 \;+\; (\nabla\cdot\widehat{\mathsf{b}})^2\right) \;+\; 6\,\langle\alpha_1^2\rangle \;-\; \frac{3}{2}\,\nabla\cdot\left[\widehat{\mathsf{b}}\,(\nabla\cdot\widehat{\mathsf{b}})\right]\right]
\end{aligned}
\tag{F 31}
$$

Here, using Eq. (11.6), we find

$$
\begin{aligned}
-\,p_\|\,\frac{\partial\Psi_2}{\partial p_\|} &= -\,2\,J\Omega\,\varrho_\|^2\,\beta_{2\|} \;+\; 2\,\frac{p_\|^2}{m}\,\varrho_\|^2\,|\boldsymbol{\kappa}|^2 \;-\; 2\,\mathbf{\Pi}_1\cdot\left(\frac{\widehat{\mathsf{b}}}{m}\times\frac{p_\|^2}{m\Omega}\,\boldsymbol{\kappa}\right), \\
-\,2\,J\,\frac{\partial\Psi_2}{\partial J} &= -\,2\,\frac{J^2}{m}\,\beta_{2\perp} \;-\; 2\,\mathbf{\Pi}_1\cdot\mathbf{v}_{\rm gc} \;-\; 2\,\mathbf{\Pi}_1\cdot\left(\frac{\widehat{\mathsf{b}}}{m}\times J\,\nabla\ln B\right),
\end{aligned}
$$

so that

$$
-\,p_\|\,\frac{\partial\Psi_2}{\partial p_\|} - 2\,J\,\frac{\partial\Psi_2}{\partial J} \;-\; 2\,\frac{p_\|^2}{m}\,\varrho_\|^2\,|\boldsymbol{\kappa}|^2 \;+\; 4\,\mathbf{\Pi}_1\cdot\mathbf{v}_{\rm gc} \;=\; -\,2\,J\Omega\,\varrho_\|^2\,\beta_{2\|} \;-\; 2\,\frac{J^2}{m}\,\beta_{2\perp}.
$$

Hence, we finally obtain

$$
\begin{aligned}
-\,6\,\beta_{2\perp} = {} & 5\,|\nabla_\perp\ln B|^2 \;-\; 2\,\langle\alpha_1^2\rangle \;+\; 4\,\widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} \;-\; 2\,\widehat{\mathsf{b}}\cdot\nabla\times\left(\widehat{\mathsf{b}}\times\nabla\ln B\right) \\
& -\; B\,\nabla\cdot\left(\frac{\nabla_\perp\ln B}{B}\right) \;-\; \boldsymbol{\kappa}\cdot\nabla\ln B \;+\; \frac{1}{2}\left(5\,\tau^2 \;-\; (\nabla\cdot\widehat{\mathsf{b}})^2\right) \\
\equiv {} & -6\,\left\{-\,\frac{1}{2}\,\tau^2 \;-\; \widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} \;+\; \langle\alpha_1^2\rangle \;+\; \frac{1}{2}\,\widehat{\mathsf{b}}\cdot\nabla\times\left(\widehat{\mathsf{b}}\times\nabla\ln B\right) \;-\; \left|\widehat{\mathsf{b}}\times\nabla\ln B\right|^2\right\},
\end{aligned}
\tag{F 32}
$$

where we used

$$
\begin{aligned}
-\,B\,\nabla\cdot\left(\frac{\nabla_\perp\ln B}{B}\right) &= -\,\widehat{\mathsf{b}}\cdot\nabla\times\left(\widehat{\mathsf{b}}\times\,\ln B\right) \;+\; \nabla\ln B\cdot\left(\boldsymbol{\kappa} \;+\; \nabla_\perp\ln B\right) \\
-\,4\,\langle\alpha_1^2\rangle &= -\,2\,\widehat{\mathsf{b}}\cdot\nabla\times\mathbf{R} \;-\; \frac{1}{2}\left[\tau^2 \;+\; \left(\nabla\cdot\widehat{\mathsf{b}}\right)^2\right],
\end{aligned}
$$

and

$$
\begin{aligned}
-\,6\,\beta_{2\|} = {} & 17\,\boldsymbol{\kappa}\cdot\nabla\ln B \;-\; \frac{B^2}{2}\,\nabla\cdot\left(\frac{\boldsymbol{\kappa}}{B^2}\right) \;-\; 18\,|\boldsymbol{\kappa}|^2 \;-\; 4\,\nabla\cdot\boldsymbol{\kappa} \\
& +\; \frac{3}{4}\left(\tau^2 \;+\; (\nabla\cdot\widehat{\mathsf{b}})^2\right) \;+\; 6\,\langle\alpha_1^2\rangle \;-\; \frac{3}{2}\,\nabla\cdot\left[\widehat{\mathsf{b}}\,(\nabla\cdot\widehat{\mathsf{b}})\right] \\
\equiv {} & -\,6\,\left\{-\,2\,\langle\alpha_1^2\rangle \;-\; 3\,\boldsymbol{\kappa}\cdot\left(\nabla\ln B \;-\; \boldsymbol{\kappa}\right) \;+\; \nabla\cdot\boldsymbol{\kappa}\right\},
\end{aligned}
\tag{F 33}
$$

where we used

$$-\frac{B^2}{2}\,\nabla\cdot\left(\frac{\boldsymbol{\kappa}}{B^2}\right) = -\,\frac{1}{2}\,\nabla\cdot\boldsymbol{\kappa} \;+\; \boldsymbol{\kappa}\cdot\nabla\ln B$$

$$6\,\langle\alpha_1^2\rangle = \frac{3}{2}\,\nabla\cdot\left[\boldsymbol{\kappa} \;-\; \widehat{\mathsf{b}}\,(\nabla\cdot\widehat{\mathsf{b}})\right] \;+\; \frac{3}{4}\left[\tau^2 \;+\; (\nabla\cdot\widehat{\mathsf{b}})^2\right].$$

Appendix G. Constraint due to the Guiding-center Toroidal Canonical Momentum

The definition of the guiding-center toroidal canonical momentum $P_{\mathrm{gc}\varphi} \equiv \mathsf{T}_{\mathrm{gc}}^{-1}P_\varphi$ as the guiding-center push-forward of the particle toroidal canonical momentum yields the expression

$$P_{\mathrm{gc}\varphi} \;=\; -\,\frac{e}{\epsilon c}\,\mathsf{T}_{\mathrm{gc}}^{-1}\psi \;+\; m\left(\frac{d_{\mathrm{gc}}\mathbf{X}}{dt} \;+\; \frac{d_{\mathrm{gc}}\boldsymbol{\rho}_{\mathrm{gc}}}{dt}\right)\cdot\left(\frac{\partial_{\mathrm{gc}}\mathbf{X}}{\partial\varphi} \;+\; \frac{\partial_{\mathrm{gc}}\boldsymbol{\rho}_{\mathrm{gc}}}{\partial\varphi}\right), \tag{G 1}$$

where the guiding-center push-forward of ψ is expressed as

$$\mathsf{T}_{\mathrm{gc}}^{-1}\psi \;=\; \psi \;+\; \epsilon\,\boldsymbol{\rho}_0\cdot\nabla\psi \;+\; \epsilon^2\left[\boldsymbol{\rho}_1\cdot\nabla\psi \;+\; \frac{1}{2}\,(\boldsymbol{\rho}_0\boldsymbol{\rho}_0):\nabla\nabla\psi\right] \;+\;\cdots, \tag{G 2}$$

the guiding-center push-forward of the particle velocity is

$$\frac{d_{\mathrm{gc}}\mathbf{X}}{dt} \;+\; \frac{d_{\mathrm{gc}}\boldsymbol{\rho}_{\mathrm{gc}}}{dt} \;=\; \left(\frac{d_0\mathbf{X}}{dt} \;+\; \Omega\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\right) \;+\; \epsilon\left(\frac{d_1\mathbf{X}}{dt} \;+\; \frac{d_0\boldsymbol{\rho}_0}{dt} \;+\; \Omega\,\frac{\partial\boldsymbol{\rho}_1}{\partial\theta}\right) + \cdots, \tag{G 3}$$

and the guiding-center push-forward of $\partial\mathbf{x}/\partial\varphi$ is

$$\frac{\partial_{\mathrm{gc}}\mathbf{X}}{\partial\varphi} \;+\; \frac{\partial_{\mathrm{gc}}\boldsymbol{\rho}_{\mathrm{gc}}}{\partial\varphi} \;=\; \mathsf{T}_{\mathrm{gc}}^{-1}\left(\frac{\partial\mathbf{x}}{\partial\varphi}\right) \;=\; \frac{\partial\mathbf{X}}{\partial\varphi} \;+\; \epsilon\,\frac{\partial\boldsymbol{\rho}_0}{\partial\varphi} \;+\;\cdots. \tag{G 4}$$

When Eqs. (G 2)-(G 4) are inserted in Eq. (G 1), we obtain the expression (up to second order in ϵ)

$$\begin{aligned} P_{\mathrm{gc}\varphi} = \left\langle\mathsf{T}_{\mathrm{gc}}^{-1}P_\varphi\right\rangle \;&+\; \left(m\Omega\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\frac{\partial\mathbf{X}}{\partial\varphi} \;-\; \frac{e}{c}\,\boldsymbol{\rho}_0\cdot\nabla\psi\right) \\ &+\epsilon\,p_\parallel\left[\widehat{\mathsf{b}}\cdot\frac{\partial\boldsymbol{\rho}_0}{\partial\varphi} \;+\; (\boldsymbol{\rho}_0\cdot\boldsymbol{\kappa})\,\widehat{\mathsf{b}}\cdot\frac{\partial\mathbf{X}}{\partial\varphi} \;+\; \left(C_{\perp\rho}\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} + C_{\rho\rho}\,\boldsymbol{\rho}_0\right)\cdot\frac{\partial\mathbf{X}}{\partial\varphi}\right] \\ &+\epsilon\,J\left[2(\mathsf{a}_2\cdot\nabla\ln B)\cdot\frac{\nabla\psi}{B} + 2\,\frac{\mathsf{a}_2}{B}:\nabla\nabla\psi - 2(\mathsf{a}_1\cdot\nabla\ln B)\cdot\frac{\partial\mathbf{X}}{\partial\varphi} + \alpha_1\,\widehat{\mathsf{b}}\cdot\frac{\partial\mathbf{X}}{\partial\varphi}\right], \end{aligned} \tag{G 5}$$

where gyroangle-dependent terms are shown explicitly up to first order in ϵ_B. Since we have the identity

$$P_{\mathrm{gc}\varphi} \;\equiv\; \left\langle\mathsf{T}_{\mathrm{gc}}^{-1}P_\varphi\right\rangle, \tag{G 6}$$

we must, therefore, show that all gyroangle-dependent terms must vanish identically.

At zeroth order in ϵ_B, we use the magnetic identity

$$\mathbf{B}\times\frac{\partial\mathbf{X}}{\partial\varphi} \;\equiv\; \nabla\psi, \tag{G 7}$$

and obtain

$$\frac{e}{c}\,\boldsymbol{\rho}_0\cdot\nabla\psi \;=\; m\Omega\,\boldsymbol{\rho}_0\cdot\widehat{\mathsf{b}}\times\frac{\partial\mathbf{X}}{\partial\varphi} \;=\; m\Omega\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\cdot\frac{\partial\mathbf{X}}{\partial\varphi},$$

and thus the gyroangle-dependent zeroth-order terms in Eq. (G 5) cancel each other out.

At first order in ϵ_B, we discuss the terms proportional to $p_\parallel$ and J in Eq. (G 5) separately. First, for the $p_\parallel$-terms, using the definitions (A 4), we find

$$C_{\perp\rho}\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} + C_{\rho\rho}\,\boldsymbol{\rho}_0 \;\equiv\; \left(\mathbf{I} \;-\; \widehat{\mathsf{b}}\,\widehat{\mathsf{b}}\right)\cdot\nabla\widehat{\mathsf{b}}\cdot\boldsymbol{\rho}_0 \;=\; \nabla\widehat{\mathsf{b}}\cdot\boldsymbol{\rho}_0 \;-\; (\boldsymbol{\kappa}\cdot\boldsymbol{\rho}_0)\,\widehat{\mathsf{b}},$$

so that

$$\left[C_{\perp\rho}\,\frac{\partial\boldsymbol{\rho}_0}{\partial\theta} + C_{\rho\rho}\,\boldsymbol{\rho}_0 \;+\; (\boldsymbol{\kappa}\cdot\boldsymbol{\rho}_0)\,\widehat{\mathsf{b}}\right]\cdot\frac{\partial\mathbf{X}}{\partial\varphi} \;=\; \frac{\partial\mathbf{X}}{\partial\varphi}\cdot\nabla\widehat{\mathsf{b}}\cdot\boldsymbol{\rho}_0 \;\equiv\; \frac{\partial\widehat{\mathsf{b}}}{\partial\varphi}\cdot\boldsymbol{\rho}_0,$$

which combines with the remaining $p_\parallel$-term in Eq. (G 5) to yield

$$\epsilon\,p_\parallel\left(\frac{\partial\widehat{\mathsf{b}}}{\partial\varphi}\cdot\boldsymbol{\rho}_0 \;+\; \widehat{\mathsf{b}}\cdot\frac{\partial\boldsymbol{\rho}_0}{\partial\varphi}\right) \;=\; \epsilon\,p_\parallel\,\frac{\partial}{\partial\varphi}\left(\widehat{\mathsf{b}}\cdot\boldsymbol{\rho}_0\right) \;\equiv\; 0.$$

Next, for the J-terms in Eq. (G 5), we use the identity

$$2\,(\mathsf{a}_2\cdot\nabla\ln B)\cdot\frac{\nabla\psi}{B} \;=\; \frac{1}{2}\left[\left(\widehat{\perp}\widehat{\perp} - \widehat{\rho}\widehat{\rho}\right)\cdot\nabla\ln B\right]\cdot\widehat{\mathsf{b}}\times\frac{\partial\mathbf{X}}{\partial\varphi} \;=\; (\mathsf{a}_1\cdot\nabla\ln B)\cdot\frac{\partial\mathbf{X}}{\partial\varphi},$$

to obtain

$$2\,\frac{\mathsf{a}_2}{B}:\nabla\nabla\psi \;-\; 2\,(\mathsf{a}_2\cdot\nabla\ln B)\cdot\frac{\nabla\psi}{B} \;+\; \alpha_1\,\widehat{\mathsf{b}}\cdot\frac{\partial\mathbf{X}}{\partial\varphi} \;=\; 2\,\mathsf{a}_2:\nabla\left(\frac{\nabla\psi}{B}\right) \;+\; \alpha_1\,\widehat{\mathsf{b}}\cdot\frac{\partial\mathbf{X}}{\partial\varphi}.$$

Here, we find

$$\begin{aligned} 2\,\mathsf{a}_2:\nabla\left(\frac{\nabla\psi}{B}\right) &= 2\,\mathsf{a}_2:\nabla\left(\widehat{\mathsf{b}}\times\frac{\partial\mathbf{X}}{\partial\varphi}\right) \;=\; \mathsf{a}_1:\nabla\left(\frac{\partial\mathbf{X}}{\partial\varphi}\right) \;+\; \frac{1}{2}\left(C_{\perp\rho} \;+\; C_{\rho\perp}\right)\widehat{\mathsf{b}}\cdot\frac{\partial\mathbf{X}}{\partial\varphi} \\ &= \mathsf{a}_1:\nabla\left(\frac{\partial\mathbf{X}}{\partial\varphi}\right) \;-\; \alpha_1\,\widehat{\mathsf{b}}\cdot\frac{\partial\mathbf{X}}{\partial\varphi}. \end{aligned}$$

which combines with the remaining J-term in Eq. (G 5) to yield

$$\epsilon\,J\;\mathsf{a}_1:\nabla\left(\frac{\partial\mathbf{X}}{\partial\varphi}\right) \;\equiv\; 0,$$

since a_1 is a symmetric matrix and $\nabla(\partial\mathbf{X}/\partial\varphi)$ is an antisymmetric matrix so that their trace vanishes.

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