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Hierarchy of second order gyrokinetic Hamiltonian models for Particle-In-Cell codes.

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Abstract. In Modern Gyrokinetic theory, choice of the reduced particle model defines polarization and magnetization effects appearing in gyrokinetic Maxwell equations. In this paper we present simplified systematic derivation of the second order Hamiltonian gyrokinetic models suitable for Particle-In-Cell simulations. Full Finite Larmor Radius(FLR) model as well as the model suitable for the *long-wavelength* limit, containing up to the second order FLR corrections are derived and compared to the model recently implemented into the Particle-In-Cell code ORB5.

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1. Introduction

Magnetized plasma represents a complex system with multi-scaled dynamics, which challenges numerical implementations. Since several decades the gyrokinetic dynamical reduction [1], [2], [3] is in the scope of the interest as one of the tools to access this multi-scaled dynamics investigation: numerically and analytically. The general gyrokinetic derivation [3] accounts background quantities gradients as well as the electromagnetic fluctuations at the same order and therefore is rather challenging. However, simplified orderings leading to the linearized polarization and magnetization in gyrokinetic Maxwell equations are often implemented in nowadays gyrokinetic codes.

The goal of this paper is to present strictly necessary for numerical implementations derivation of the reduced particle dynamics and to build up the hierarchy of the most common reduced particle models.

Modern gyrokinetic theory considered as a field theory gives access to derivation of a self-consistently coupled gyrokinetic Maxwell-Vlasov equations. The reduced particle model defines the gyrokinetic Vlasov equation, reconstructed via particles characteristics. The reduced particle dynamics affects the reduced Maxwell equations via polarization and magnetization contributions, that link can be systematically established within the first principle derivation from the gyrokinetic Lagrangian [4], [5]. Details of such a derivation for the particle models containing up to the second order Finite Larmor Radius (FLR) corrections can be found in [6].

This paper focusses on the generalised and detailed derivation of the Hamiltonian models for gyrokinetic particle dynamics, which has been presented in a simplified form into the Appendix A of [6]. A detailed comparison has been provided between the second order FLR model following from the general gyrokinetic derivation and the one recently implemented into the Particle-In-Cell (PIC) code ORB5 [7].

This paper is organised as follows: in Sec. 2 we remind the main idea of the gyrokinetic reduction, in Sec. 3 we set up the general framework for the change of coordinates and the reduced dynamics derivation, in Sec. 4 we present the Hamiltonian models derivation: first in the case with full series of the Finite Larmor Radius (FLR) corrections and then in the *long-wavelength* approximation. The second order (with respect to the amplitudes of fluctuating fields) Maxwell-Vlasov gyrokinetic model corresponding to the full FLR gyrokinetic particle model and the model containing the second order FLR corrections suitable for the *long-wavelength* approximation are currently implemented in PIC code ORB5.

2. Gyrokinetic dynamical reduction

In magnetised plasmas presence of strong magnetic field induces scales of motion separation. Particle's dynamics is decomposed into the fast rotation around the magnetic field lines and slow drift motion in the perpendicular direction. The cyclotron frequency $\Omega = eB/mc$, where e and m are, respectively, the charge and mass of particles,

B is the magnetic field amplitude and c is the speed of light, sets the scale of gyromotion.

The gyromotion is described by a fast gyroangle variable θ to which corresponds a canonically conjugated slowly varying magnetic moment μ. At the lowest order

$$\mu = mv_\perp^2/2B, \tag{1}$$

where $v_\perp$ is the perpendicular velocity of particles with respect to the magnetic field lines. In slab magnetic geometry μ is an exact dynamical invariant. However magnetic curvature effects as well as the presence of electromagnetic fluctuations destroys that exact invariance. The gyrokinetic dynamical reduction uses the fact that averaged over long times magnetic moment still being conserved, i.e. $\langle\dot{\mu}\rangle_t = 0$.

The goal of the gyrokinetic dynamical reduction consists in building up a new set of phase space variables, such that θ dependence is completely uncoupled and μ has a trivial dynamics, i.e. $\dot{\mu} = 0$. Therefore, the reduced particle dynamics is described on the 4 dimensional phase space with variables $(\mathbf{X}, p)$, where $\mathbf{X}$ represents the reduced particle position and p is the corresponding scalar momentum coordinate. This change of coordinate is constructed via perturbative series of near-identity phase space transformations, i.e. these transformations are invertible at each step of the perturbative procedure. The reduced position $\mathbf{X}$ has a simple geometrical meaning: it is the instantaneous center of the fastest particle's rotation around the magnetic field line. Therefore, the gyrokinetic coordinate transformation is a shift between the initial particle coordinate and the instantaneous center of its rotation. Performing numerical simulations on the 4 dimensional phase space instead of the 6 dimensional one aims to reduce numerical costs.

The dynamical reduction can be organized in one or two steps. Within the one step procedure, the contributions from the background geometry non-uniformities and electromagnetic fluctuations to the breaking of the magnetic momentum conservation are taken into account simultaneously. The two step procedure allows to treat those effects at the separate stages, which may have some advantages for making a direct link between the coordinate transformation and polarization effects it induces on the reduced particle and field dynamics. Here we consider the two-step procedure in order to make a clear separation between the polarization contributions associated to each of those transformations at the lowest order. Within the two step procedure, a small parameter is associated to each transformation: for the *guiding-center* $\epsilon_B = \rho_{th}/L_B$, where ρ_{th} is thermal Larmor radius of particle and $L_B = \nabla B/B$ sets the spatial scale for background magnetic field variation, and $\epsilon_\delta = (k_\perp \rho_{th})\ e\phi/T$ for the *gyrocenter*. Following the gyrokinetic code ordering, we consider in this work that $\epsilon_B \ll \epsilon_\delta$, i.e. all the background gradient effects are of the superior order with respect to the amplitudes of the fluctuations.

As a perturbative theory, each of the coordinate transformations: *the guiding-center* and *the gyrocenter* represent an infinite series of corrections ordered accordingly to the corresponding small parameter: ϵ_B or ϵ_δ. From the point of view of spatial components of the coordinate transformation, it means that the exact gyrokinetic coordinate transformation contains an infinite series of polarization displacements. In this work we provide an explicit derivation of the reduced particle dynamics at the lowest orders of both transformations. In that case, spatial components of both phase space transformations: *guiding-center* and *gyrocenter* represent a shift between the initial non-reduced particle position $\mathbf{x}$ and the reduced gyrocenter position $\mathbf{X}$:

$$\mathbf{x} = \mathbf{X} + \boldsymbol{\rho}_0(\mathbf{X}, \mu, \theta) + \epsilon_\delta \boldsymbol{\rho}_1(\mathbf{X}, \mu, \theta), \tag{2}$$

where we have introduced polarization displacements of two kind: $\boldsymbol{\rho}_0$ corresponding to the lowest order *guiding-center* reduction and $\boldsymbol{\rho}_1$ corresponding to the lowest order of the *gyrocenter* reduction.

The lowest order guiding-center displacement is given by:

$$\boldsymbol{\rho}_0 \equiv \frac{mc}{e}\sqrt{\frac{2\mu}{mB}}\,\widehat{\boldsymbol{\rho}} \equiv \rho_0 \widehat{\boldsymbol{\rho}} \sim \mathcal{O}(\epsilon_B^0), \tag{3}$$

where $\widehat{\boldsymbol{\rho}}$ is the unitary vector in the plane perpendicular to the background magnetic field; the magnitude of magnetic field B is evaluated at the reduced position $\mathbf{X}$. The general gyrokinetic derivation comes up with a result that all the following *guiding-center* polarization displacements are at least of the order $\mathcal{O}(\epsilon_B)$ or higher (see, for example the Eq. 36 in [8] or the Eqns. 63 and 66 in [9]), this is why we are not considering them here.

In the same time, the lowest order gyrocenter displacement:

$$\boldsymbol{\rho}_1 = \frac{mc^2}{B^2}\boldsymbol{\nabla}_\perp \left(\phi_1(\mathbf{X}) - \frac{p_z}{mc}A_{1\|}(\mathbf{X})\right) \sim \mathcal{O}(\epsilon_\delta), \tag{4}$$

where p_z is the gyrocenter scalar canonical momentum coordinate related to the parallel guiding-center momentum accordingly to the Eq. (10). In this work we consider the gyrokinetic coordinate transformation in two cases: in the Sec. 3 we present the transformation containing all the Finite Larmor Radius (FLR) corrections, i.e. from the point of view of functional dependencies of electrostatic potentials containing corrections of all orders related to the *guiding-center* transformation $\mathbf{x} = \mathbf{X} + \boldsymbol{\rho}_0$.

Then in the Sec. 5.2 we explicit the change of coordinate at the lowest FLR order, which corresponds from the physical point of view to the *long-wavelenght* approximation with $k_\perp \rho_{\text{th}} \ll 1$. We show that in this limit the gyrocenter phase space transformation affects the spatial coordinate only, while the velocity phase space coordinates (p, μ, θ) remain unchanged, so it acts only as a shift between the guiding-center $\mathbf{X} + \boldsymbol{\rho}_0$ and the gyrocenter $\mathbf{X} + \boldsymbol{\rho}_0 + \epsilon_\delta \boldsymbol{\rho}_1$ positions.

3. Phase-space perturbative procedure

In modern gyrokinetic theory, definition of new phase-space coordinates is done within common perturbative procedure together with the derivation of the reduced dynamics. At the first step, the *guiding-center* dynamical reduction starts from the local particle coordinates $(\mathbf{x}, \mathbf{v})$. To access those coordinates, one needs to define two vector basis: the static one and the dynamical one. The static basis is related to the magnetic field line and the dynamical one rotates with the particle. As the static basis we choose the natural Frenet triad : the unitary magnetic field vector $\widehat{\mathbf{b}} = \mathbf{B}/B$, the normalized curvature vector $\widehat{\mathbf{b}}_1 = \widehat{\mathbf{b}} \cdot \boldsymbol{\nabla}\widehat{\mathbf{b}}/|\widehat{\mathbf{b}} \cdot \boldsymbol{\nabla}\widehat{\mathbf{b}}|$ and $\widehat{\mathbf{b}}_2 = \widehat{\mathbf{b}} \times \widehat{\mathbf{b}}_1$. Then, the dynamical basis is defined from the static one as follows:

$$\widehat{\boldsymbol{\rho}} = \widehat{\mathbf{b}}_1 \cos\theta - \widehat{\mathbf{b}}_2 \sin\theta, \quad \widehat{\perp} = -\widehat{\mathbf{b}}_1 \sin\theta - \widehat{\mathbf{b}}_2 \cos\theta, \tag{5}$$

where $\widehat{\boldsymbol{\rho}}$ is used for definition of the *guiding-center* displacement $\boldsymbol{\rho}_0$ in the Eq. (3) and therefore the local particle velocity can be decomposed in the following way:

$$\mathbf{v} = v_\| \widehat{\mathbf{b}} + \sqrt{\frac{2\mu B}{m}}\,\widehat{\perp}. \tag{6}$$

At the lowest order, the guiding-center transformation is defined as follows: the particle space coordinate is decomposed as $\mathbf{x} = \mathbf{X} + \boldsymbol{\rho}_0(\mathbf{X}, \mu, \theta)$, with $\mathbf{X}$ the reduced particle position and $\boldsymbol{\rho}_0$ the lowest order guiding-center polarization shift; the scalar momentum coordinate is the parallel kinetic momentum $p_\| = mv_\|$; μ is the lowest order magnetic momentum given by the Eq. (1) and θ is the fast angle of rotation.

Since all kind of the invertible coordinate transformations are allowed for expression of the Lagrangian dynamics, we write the expression for *the guiding-center* phase space Lagrangian 1-form in the $\left(\mathbf{X}, p_\|, \mu, \theta\right)$ coordinates:

$$L_{\mathrm{gc}}\left(\mathbf{X}, p_\|, \mu, \theta\right) = \frac{e}{c}\mathbf{A}^* \cdot \dot{\mathbf{X}} + \frac{mc}{e}\mu\,\dot{\theta} - H_{\mathrm{gc}}, \tag{7}$$

where the symplectic part contains the modified magnetic potential:

$$\mathbf{A}^* = \mathbf{A} + \frac{c}{e}\,p_\|\widehat{\mathbf{b}}. \tag{8}$$

The guiding-center Hamiltonian is given by:

$$H_{\mathrm{gc}} = \frac{p_\|^2}{2m} + \mu B. \tag{9}$$

The L_{gc} Lagrangian is the starting point of the derivation. At the next step, we perturb that expression with first order fluctuating time-dependent electromagnetic fields ϕ_1 and $A_{1\|}$ both $\sim \mathcal{O}(\epsilon_\delta)$. Remark that in our derivation the perpendicular part of the perturbed magnetic potential is absent, which corresponds to the choice of considering the perpendicular component of the perturbed magnetic field only: $\mathbf{B}_1 = \boldsymbol{\nabla} \times A_{1\|}\widehat{\mathbf{b}}$. This approximation is implemented into the electromagnetic Particle-In-Cell code ORB5.

In order to take into the account then eventual time-dependence of perturbed electromagnetic potentials $A_{1\|}$ and ϕ_1 we extend the phase space from 6 to 8 dimensions. Therefore, formally the *gyrocenter* dynamical reduction is performed on the 8-dimensional phase space where (t, w) are canonically conjugated: t time and w energy variables. This extension of the phase space is a standard for dynamical systems procedure of autonomization (see for example [10]). From the physical point of view, relevant reduced dynamics is still be performed on the 4 dimensional part of the *gyrocenter* phase space with coordinates $(\mathbf{X}, p_z)$, where

$$p_z = mv_\| + \frac{e}{c}A_{1\|}(\mathbf{X} + \boldsymbol{\rho}_0) \tag{10}$$

is the gyrocenter canonical momentum.

The perturbed *guiding-center* phase-space Lagrangian is given by:

$$\widetilde{L}\left(\mathbf{X}, p_z, \mu, \theta; t, w\right) = \left(\frac{e}{c}\mathbf{A} + p_z\widehat{\mathbf{b}}\right)\dot{\mathbf{X}} + \frac{mc}{e}\mu\dot{\theta} - \left(\frac{p_z}{2m} + \mu B + e\phi_1(\mathbf{X}+\boldsymbol{\rho}_0)\right.$$
$$\left. - \frac{e\ p_z}{2m}A_{1\|}(\mathbf{X}+\boldsymbol{\rho}_0) + \frac{1}{2m}\left(\frac{e}{c}\right)^2 A_{1\|}^2(\mathbf{X}+\boldsymbol{\rho}_0) - w\right), \tag{11}$$

where $\mathbf{A}$ is the background vector potential, and $\widehat{\mathbf{b}}$ is the unitary vector associated to the background magnetic field $\mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A}$. As all the background quantities $\mathbf{A}$, $\widehat{\mathbf{b}}$ and B are evaluated into the reduced gyrocenter position $\mathbf{X}$, while the perturbative electromagnetic potentials $A_{1\|}$ and ϕ_1 are evaluated into the *guiding-center* position $\mathbf{X}+\boldsymbol{\rho}_0$, i.e. containing the gyrophase dependencies through the $\boldsymbol{\rho}_0$. The two first terms in the Eq. (11) represent the non-perturbed symplectic part and the last term is the perturbed Hamiltonian of the system. Keeping the symplectic part gyrophase-independent is possible within the p_z-representation (10) of the dynamics. In that representation all gyrophase-dependent terms are contained into the expression for the Hamiltonian. This is one of the common choices for the Particle-In-Cell simulations since it avoids appearance of the inductive electric field (the explicit time-derivative of the perturbative magnetic potential $A_{1\|}$) into the particle characteristics.

In the next section we show how to eliminate the gyrophase-dependencies induced by the perturbed electromagnetic potentials with using the Lie-transform near-identity transformation at the first order with respect to the small parameter ϵ_δ. We also explicit the connection between the choice of the displacements $\boldsymbol{\rho}_0$, $\boldsymbol{\rho}_1$ and elimination of the gyrophase-dependencies into the dynamics.

4. Full FLR Hamiltonian model

In this section we build up a near-identity phase-space change of variables aiming to eliminate gyrophase-dependencies from the perturbative electromagnetic potentials $A_{1\|}$ and ϕ_1 into the dynamics generated by the phase-space Lagrangian (11). We also show the link between this change of coordinate and corrections appearing into the expression for the reduced Hamiltonian.

Since in the p_z representation of dynamics the symplectic part of the phase-space Lagrangian is unperturbed, the *gyrocenter* change of coordinates will induce effects only into its Hamiltonian part.

To define that change of coordinates, we derive the expression for the Poisson Bracket, which can be obtained from the symplectic part of the perturbed Lagrangian (11):

$$\{F, G\} = \frac{e}{mc}\left(\frac{\partial F}{\partial\theta}\frac{\partial G}{\partial\mu} - \frac{\partial F}{\partial\mu}\frac{\partial G}{\partial\theta}\right) + \frac{\mathbf{B}^*}{B_\|^*}\cdot\left(\boldsymbol{\nabla}F\frac{\partial G}{\partial p_z} - \frac{\partial F}{\partial p_z}\boldsymbol{\nabla}G\right)$$
$$- \frac{c\widehat{\mathbf{b}}}{eB_\|^*}\cdot(\boldsymbol{\nabla}F\times\boldsymbol{\nabla}G) - \frac{\partial F}{\partial w}\frac{\partial G}{\partial t} + \frac{\partial F}{\partial t}\frac{\partial G}{\partial w}, \tag{12}$$

where $\mathbf{B}^* = \mathbf{B} + \frac{e}{c} p_z \boldsymbol{\nabla} \times \widehat{\mathbf{b}}$ and $B^*_\| = \mathbf{B}^* \cdot \widehat{\mathbf{b}}$. The first three terms of that bracket are ordered following the formal ordering introduced by Newcomb [11]: $\epsilon_B \sim e^{-1}$. So the first term generates the fastest scale of motion, the second one is related to the drifts along the magnetic field lines, while $\mathbf{B}^*/B^*_\| \sim \widehat{\mathbf{b}}$; and the last one is associated with the slowest perpendicular drifts. The last two canonical terms corresponds to the extension of the phase space up to 8 dimensions.

Following the p_z-representation of the Lagrangian defined in the Eq. (11), the second order gyrocenter Hamiltonian is:

$$H = H_0 + e\ \psi_1(\mathbf{X} + \boldsymbol{\rho}_0(\mu,\theta), p_z) + \frac{1}{2m}\left(\frac{e}{c}\right)^2 A_{1\|}(\mathbf{X} + \boldsymbol{\rho}_0(\mu,\theta))^2, \tag{13}$$

where the unperturbed guiding-center Hamiltonian now writes as:

$$H_0 = \frac{p_z^2}{2m} + \mu B \tag{14}$$

and

$$\psi_1(\mathbf{X} + \boldsymbol{\rho}_0(\mu,\theta), p_z) \equiv\ \phi_1(\mathbf{X} + \boldsymbol{\rho}_0) - \frac{1}{mc}\ p_z\ A_{1\|}(\mathbf{X} + \boldsymbol{\rho}_0) \tag{15}$$

is the linear perturbed gyrocenter potential. Remark that the *guiding-center* displacement $\boldsymbol{\rho}_0$ given by the Eq. (3) is formally depending on the phase-space coordinates $(\mathbf{X}, \mu, \theta)$. Because all the dynamical fields automatically depend on the reduced position $\mathbf{X}$ not only through the guiding-center displacement field $\boldsymbol{\rho}_0$, in what follows we keep in mind the $\boldsymbol{\rho}_0$ dependence in the velocity part of the phase-space coordinates (μ, θ) without specifying its spatial dependency. This is justified by the fact that we are performing the calculation on the lowest order with respect to the *guiding-center* displacement $\boldsymbol{\rho}_0$. Derivation of $\boldsymbol{\rho}_0$ with respect to the spatial coordinate $\mathbf{X}$ would lead to appearance of the $\nabla B/B$ coefficient, which would in its turn lead to appearance of the $\mathcal{O}(\epsilon_B)$ terms, which are neglected here anyway. To make formulas appearing more compact we omit writing the functional dependencies of the displacement $\boldsymbol{\rho}_0$ in the following text explicitely but we keep in mind its (μ, θ) dependencies.

4.1. Gyrocenter phase-space coordinate transformation

In order to eliminate the gyrophase dependence of the Hamiltonian H, we perform a Lie transform which maps the guiding-center coordinates $(\mathbf{X}, p_z, \mu, \theta)$ into the gyrocenter ones. Up to the first order, this change of coordinates is defined as follows:

$$e^{-\pounds_{S_1}}(\mathbf{X} + \boldsymbol{\rho}_0) = \mathbf{X} + \boldsymbol{\rho}_0 - \epsilon_\delta\{S_1, \mathbf{X} + \boldsymbol{\rho}_0\} \tag{16}$$

$$e^{-\pounds_{S_1}} p_z = p_z - \epsilon_\delta\{S_1, p_z\} \tag{17}$$

$$e^{-\pounds_{S_1}} \mu = \mu - \epsilon_\delta\{S_1, \mu\} \tag{18}$$

$$e^{-\pounds_{S_1}} \theta = \theta - \epsilon_\delta\{S_1, \theta\}, \tag{19}$$

where S_1 is the generating function defining the transformation at the first order.

We define the first order gyrocenter displacement as the shift between the guiding-center and the gyrocenter positions:

$$\boldsymbol{\rho}_1 = -\epsilon_\delta \{S_1, \mathbf{X} + \boldsymbol{\rho}_0\}, \tag{20}$$

therefore

$$e^{-\pounds_{S_1}}(\mathbf{X} + \boldsymbol{\rho}_0) = \mathbf{X} + \boldsymbol{\rho}_0 + \boldsymbol{\rho}_1. \tag{21}$$

4.2. Full FLR gyrocenter dynamics

In the same time, the Hamiltonian expressed in new coordinates, up to the second order in ϵ_δ is:

$$\begin{aligned}\overline{H} = e^{-\pounds_{S_2}} e^{-\pounds_{S_1}} H &= H_0 - \epsilon_\delta \{S_1, H_0\} + \frac{1}{2}\epsilon_\delta^2 \{S_1, \{S_1, H_0\}\} + \epsilon_\delta^2 \{S_2, H_0\} \\ &+ \epsilon_\delta \psi_1(\mathbf{X} + \boldsymbol{\rho}_0; p_z) - \epsilon_\delta^2 \{S_1, \psi_1(\mathbf{X} + \boldsymbol{\rho}_0; p_z)\} \\ &+ \epsilon_\delta^2 \frac{1}{2m}\left(\frac{e}{c}\right)^2 A_{1\|}(\mathbf{X} + \boldsymbol{\rho}_0)^2 + \mathcal{O}(\epsilon_\delta^3),\end{aligned} \tag{22}$$

where S_1 is the same generating function as in the Eqns. (16-19). Remark that from the point of view of the Hamiltonian, S_1 is removing the gyrophase dependence at the orders ϵ_δ and ϵ_δ^2. The generating function S_2 is defined such that it removes the gyroangle dependence from the order ϵ_δ^2 terms. The expression of the generating function S_2 is defined at the next order of perturbative procedure and involves terms of $\mathcal{O}(\epsilon_\delta^3)$.

The expression for S_1 is obtained from the condition that the gyrophase dependent part of linear electromagnetic perturbation $\widetilde{\psi}_1$ is removed from the lowest order gyrocenter Hamiltonian:

$$\{S_1, H_0\} = e\,\widetilde{\psi}_1(\mathbf{X} + \boldsymbol{\rho}_0, p_z) = e\psi_1(\mathbf{X} + \boldsymbol{\rho}_0, p_z) - e\mathcal{J}_0(\psi_1(\mathbf{X} + \boldsymbol{\rho}_0, p_z)) \tag{23}$$

and the gyroaveraged quantities are defined as follows:

$$(\mathcal{J}_0\psi)(\mathbf{X}, p_z, \mu) = \frac{1}{2\pi}\int_0^{2\pi} \psi(\mathbf{X} + \boldsymbol{\rho}_0, p_z)\, d\theta. \tag{24}$$

Therefore, the second order contribution:

$$\{S_1, \{S_1, H_0\}\} = \{S_1, \widetilde{\psi}_1(\mathbf{X} + \boldsymbol{\rho}_0; p_z)\} \tag{25}$$

.

By taking into the account the explicit expression for the guiding-center Poisson bracket (12) at the lowest order:

$$\{F, G\} = \frac{e}{mc}\frac{\partial}{\partial\theta}\left(F\frac{\partial G}{\partial\mu}\right) - \frac{e}{mc}\frac{\partial}{\partial\mu}\left(F\frac{\partial G}{\partial\theta}\right), \tag{26}$$

the condition (23) becomes:

$$\frac{e}{mc}\frac{\partial S_1}{\partial\theta}\frac{\partial H_{\rm gc}}{\partial\mu} = \frac{eB}{mc}\frac{\partial S_1}{\partial\theta} = e\,\widetilde{\psi}_1(\mathbf{X} + \boldsymbol{\rho}_0; p_z), \tag{27}$$

and therefore the generating function is:

$$S_1 = \frac{e}{\Omega}\int d\theta\, \widetilde{\psi}_1(\mathbf{X} + \boldsymbol{\rho}_0; p_z), \tag{28}$$

which means that this function has a fluctuating part only, i.e. $(\mathcal{J}_0 S_1) = 0$ and $S_1 = S_1(\mathbf{X} + \boldsymbol{\rho}_0; p_z)$.

Since S_2 removes fluctuating parts from the second order terms, we only need to evaluate the corresponding gyroaveraged contributions. With taking into the account the Eq. (25) and the fact that S_1 is purely fluctuating function: $\mathcal{J}_0(\{S_1, \psi_1\}) = \mathcal{J}_0\left(\{S_1, \widetilde{\psi}_1\}\right)$ we obtain a partial cancellation of the second order term $\mathcal{O}(\epsilon_\delta^2)$:

$$\begin{aligned}\frac{1}{2}\mathcal{J}_0(\{S_1, \{S_1, H_0\}\}) &- \mathcal{J}_0(\{S_1, \psi_1(\mathbf{X} + \boldsymbol{\rho}_0; p_z)\}) \\ &= -\frac{1}{2}\mathcal{J}_0(\{S_1, \psi_1(\mathbf{X} + \boldsymbol{\rho}_0; p_z)\})\end{aligned} \tag{29}$$

Finally, we get the expression for the second order Hamiltonian containing the *guiding-center* FLR corrections at all orders:

$$\begin{aligned}\overline{H}^{\rm full} &= \frac{p_z^2}{2m} + \mu B + \epsilon_\delta\left(e\mathcal{J}_0(\phi_1(\mathbf{X} + \boldsymbol{\rho}_0))\right. \quad (30)\\ &- \left.\frac{e}{mc}\, p_z\, \mathcal{J}_0\left(A_{1\|}(\mathbf{X} + \boldsymbol{\rho}_0)\right)\right) + \epsilon_\delta^2\frac{1}{2m}\left(\frac{e}{c}\right)^2 \mathcal{J}_0\left(A_{1\|}(\mathbf{X} + \boldsymbol{\rho}_0)^2\right)\\ &- \epsilon_\delta^2\frac{e}{2}\mathcal{J}_0\left(\{S_1, \widetilde{\psi}_1(\mathbf{X} + \boldsymbol{\rho}_0, p_z)\}\right). \quad (31)\end{aligned}$$

With using the expression for the lowest order Poisson bracket given by the Eq. (26):

$$\begin{aligned}\{S_1, \widetilde{\psi}_1(\mathbf{X} + \boldsymbol{\rho}_0; p_z)\} &= \frac{\partial}{\partial\mu}\left(\widetilde{\psi}_1(\mathbf{X} + \boldsymbol{\rho}_0; p_z)\frac{\partial S_1}{\partial\theta}\right)\\ &- \frac{\partial}{\partial\theta}\left(\widetilde{\psi}_1(\mathbf{X} + \boldsymbol{\rho}_0; p_z)\frac{\partial S_1}{\partial\mu}\right)\end{aligned}$$

with using that $\partial_\theta S_1 = \widetilde{\psi}_1(\mathbf{X} + \boldsymbol{\rho}_0; p_z)$, after gyroaveraging, we get:

$$\mathcal{J}_0\left(\{S_1, \widetilde{\psi}_1(\mathbf{X} + \boldsymbol{\rho}_0; p_z)\}\right) = \partial_\mu \mathcal{J}_0\left(\widetilde{\psi}(\mathbf{X} + \boldsymbol{\rho}_0; p_z)^2\right). \tag{32}$$

$$\begin{aligned}\overline{H}^{\rm full} &= \frac{p_z^2}{2m} + \mu B + \epsilon_\delta\left(e\mathcal{J}_0(\phi_1(\mathbf{X} + \boldsymbol{\rho}_0))\right.\\ &- \left.\frac{e}{mc}\, p_z\, \mathcal{J}_0\left(A_{1\|}(\mathbf{X} + \boldsymbol{\rho}_0)\right)\right) + \epsilon_\delta^2\frac{1}{2m}\left(\frac{e}{c}\right)^2 \mathcal{J}_0\left(A_{1\|}(\mathbf{X} + \boldsymbol{\rho}_0)^2\right)\\ &- \epsilon_\delta^2\frac{e}{2mc}\partial_\mu\mathcal{J}_0\left(\widetilde{\psi}(\mathbf{X} + \boldsymbol{\rho}_0; p_z)^2\right)\end{aligned} \tag{33}$$

This result corresponds to the derivation given in [12] in the electrostatic limit and to the expression obtained in the slab magnetic geometry in [13].

5. Hamiltonian model in *long-wavelength* approximation

The *long-wavelenght* approximation with $k_\perp \rho_{\rm th} \ll 1$ is implemented into the gyrokinetic codes as an useful tool for investigation of the MHD modes, it is also suitable for studies of turbulence generated by interaction of modes with low toroidal numbers. As have been shown in the latest linear electromagnetic benchmark [14], the *long-wavelength* approximation implemented into the ORB5 code allows to treat modes with $k_\perp \rho_{\rm th} < 0.6$. From the point of view of the gyrokinetic dynamical reduction, the *long-wavelength* limit means that only the lowest order *guiding-center* FLR effects are included into the derivation. The four-point gyroaverage approximation [15] is consistent with the *long-wavelength* approximation.

Recently a full FLR solver for the Poisson equation has been implemented in ORB5 [Julien PhD]. Preliminary results shown that the new algorithm is 2 times slower then the long-wavelength solver. This is mostly due to the need for additional integration points for the gyroaverage algorithm as it was already shown in [16].

In this section we show how to obtain that simplified model in the framework of the general derivation. There are two different ways to proceed. First of all, one can perform the first order FLR series truncation directly on the expression of the second order electrostatic potential given by the Eq. (32). Another possibility is to follow the main steps of the general derivation with introducing the FLR truncation at each step: starting with the expression for the generating function S_1, getting the corresponding *gyrocenter* change of coordinates and finally the expression for the simplified Hamiltonian. In the Sec. 5.2 we expose the main steps of this derivation.

We start with obtaining the *long wavelenght* limit model via the direct full FLR model truncation.

5.1. Direct full FLR model truncation

Here we evaluate the lowest order FLR contribution to the second order term of the Hamiltonian (33). We start with decomposing the first order fluctuating electromagnetic potential into the FLR series:

$$\widetilde{\psi}_1(\mathbf{X}+\boldsymbol{\rho}_0, p_z) = \boldsymbol{\rho}_0 \cdot \boldsymbol{\nabla}\psi_1(\mathbf{X}, p_z) + \boldsymbol{\rho}_0\boldsymbol{\rho}_0 : \boldsymbol{\nabla}\boldsymbol{\nabla}\psi_1(\mathbf{X}, p_z) + \dots \tag{34}$$

In the long-wavelength limit we keep the first term only and we calculate:

$$\begin{aligned}\frac{\partial}{\partial\mu}\mathcal{J}_0\left(\widetilde{\psi}_1\left(\mathbf{X}+\boldsymbol{\rho}_0(\mu,\theta);p_z\right)^2\right) &= \frac{\partial}{\partial\mu}\mathcal{J}_0\left(\left|\boldsymbol{\rho}_0\cdot\boldsymbol{\nabla}\psi_1(\mathbf{X},p_z)\right|^2\right) = \\ = \frac{\partial}{\partial\mu}\left(\rho_0^2\right)\mathcal{J}_0\left(\widehat{\boldsymbol{\rho}}\widehat{\boldsymbol{\rho}} : \boldsymbol{\nabla}\psi_1(\mathbf{X},p_z)\boldsymbol{\nabla}\psi_1(\mathbf{X},p_z)\right) &= \left(\frac{c}{e}\right)^2\frac{1}{B}\left|\boldsymbol{\nabla}_\perp\psi_1(\mathbf{X},p_z)\right|^2,\end{aligned} \tag{35}$$

where we have used the definition (3), the fact that $\frac{1}{2}\frac{\partial\rho_0^2}{\partial\mu} = \frac{c^2 m}{e^2 B}$ and the dyadic tensors property $\mathcal{J}_0\left(\widehat{\boldsymbol{\rho}}\widehat{\boldsymbol{\rho}}\right) = \frac{1}{2}\left(\widehat{\mathbf{b}}_1\widehat{\mathbf{b}}_1 + \widehat{\mathbf{b}}_2\widehat{\mathbf{b}}_2\right) = \frac{1}{2}\mathbf{1}_\perp$.

The magnetic term of the second order is obtained from:

$$\begin{aligned}\mathcal{J}_0\left(A_{1\|}(\mathbf{X}+\boldsymbol{\rho}_0)^2\right) &= \mathcal{J}_0\left(\left(A_{1\|}^2(\mathbf{X}) + \boldsymbol{\rho}_0\cdot\boldsymbol{\nabla}A_{1\|}(\mathbf{X}) + \frac{1}{2}\boldsymbol{\rho}_0\boldsymbol{\rho}_0 : \boldsymbol{\nabla}\boldsymbol{\nabla}A_{1\|}(\mathbf{X})\right)^2\right) \\ = A_{1\|}^2(\mathbf{X}) + m\left(\frac{c}{e}\right)^2\frac{\mu}{B}\left|\boldsymbol{\nabla}_\perp A_{1\|}(\mathbf{X})\right|^2 &+ m\left(\frac{c}{e}\right)^2\frac{\mu}{B}A_{1\|}(\mathbf{X})\ \boldsymbol{\nabla}_\perp^2 A_{1\|}(\mathbf{X}).\end{aligned} \tag{36}$$

We remark that the second term is missing into the ORB5 model [6], which corresponds to the slab geometry result obtained in [13].

$$
\begin{aligned}
\overline{H}^{\mathrm{FLR}} &= \frac{p_z^2}{2m} + \mu B + \epsilon_\delta \left(e\ \mathcal{J}_0\left(\phi_1(\mathbf{X}+\boldsymbol{\rho}_0)\right) - \frac{e}{mc}\ p_z\ \mathcal{J}_0\left(A_{1\|}(\mathbf{X}+\boldsymbol{\rho}_0)\right)\right) \\
&+ \epsilon_\delta^2 \left(\frac{1}{2m}\left(\frac{e}{c}\right)^2 A_{1\|}^2(\mathbf{X}) + m\left(\frac{c}{e}\right)^2\ \frac{\mu}{B}\left|\boldsymbol{\nabla}_\perp A_{1\|}(\mathbf{X})\right|^2\right) \qquad (37)\\
&+ \epsilon_\delta^2 \left(m\left(\frac{c}{e}\right)^2\ \frac{\mu}{B} A_{1\|}(\mathbf{X})\ \boldsymbol{\nabla}_\perp^2 A_{1\|}(\mathbf{X}) - \frac{mc^2}{2B^2}\left|\boldsymbol{\nabla}_\perp\phi_1(\mathbf{X}) - \frac{e}{c}\ p_z \boldsymbol{\nabla}_\perp A_{1\|}(\mathbf{X})\right|^2\right),
\end{aligned}
$$

5.2. Gyrocenter coordinate transformation in long-wavelength approximation

In this section we derive the truncated Hamiltonian model (37) by performing the *gyrocenter* coordinate transformation (16-19) at the lowest FLR order. To that purpose, we are taking into the account only the lowest order FLR correction to the generating function S_1. Since the lowest order FLR correction to the fluctuating electromagnetic potential is $\widetilde{\psi}_1\left(\mathbf{X}+\boldsymbol{\rho}_0\right) = \rho_0 \widehat{\boldsymbol{\rho}} \cdot \boldsymbol{\nabla}\psi_1(\mathbf{X})$, from the Eq. (28) with using the property of rotating basis vectors $\widehat{\boldsymbol{\rho}} = \int d\theta\ \widehat{\perp}$, we get:

$$
S_1 = \frac{mc}{B}\rho_0\ \widehat{\perp}\cdot\boldsymbol{\nabla}\psi_1(\mathbf{X}). \qquad (38)
$$

Now we calculate the corresponding gyrocenter displacement $\boldsymbol{\rho}_1$ with using the definition (20). Taking into account the lowest order Poisson bracket (26):

$$
\boldsymbol{\rho}_1 = -\left\{S_1, \mathbf{X}+\boldsymbol{\rho}_0\right\} = -\frac{e}{mc}\left(\frac{\partial S_1}{\partial\theta}\frac{\partial\boldsymbol{\rho}_0}{\partial\mu} - \frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\frac{\partial S_1}{\partial\mu}\right).
$$

From the definition of rotating basis vectors (5), and $\partial_\mu\rho_0^2 = \frac{2mc^2}{e^2B}$, we have:

$$
\frac{e}{mc}\frac{\partial S_1}{\partial\theta}\frac{\partial\boldsymbol{\rho}_0}{\partial\mu} = \frac{mc^2}{eB^2}\ \widehat{\boldsymbol{\rho}}\widehat{\boldsymbol{\rho}}\cdot\boldsymbol{\nabla}\psi_1 \quad\text{and}\quad -\frac{e}{mc}\frac{\partial\boldsymbol{\rho}_0}{\partial\theta}\frac{\partial S_1}{\partial\mu} = \frac{mc^2}{eB^2}\ \widehat{\perp}\widehat{\perp}\cdot\boldsymbol{\nabla}\psi_1.
$$

By taking into the account definition of the dyadic tensor $\mathbf{1}_\perp \equiv \widehat{\boldsymbol{\rho}}\widehat{\boldsymbol{\rho}} + \widehat{\perp}\widehat{\perp}$, the expression for the first order gyrocenter displacement in the *long wavelength approximation* is:

$$
\boldsymbol{\rho}_1 = -\frac{mc^2}{eB^2}\boldsymbol{\nabla}_\perp\psi_1. \qquad (39)
$$

At the lowest FLR order of the *gyrocenter* phase-space transformation only the spatial coordinate is affected. Velocity space coordinates (p_z, μ, θ) remain unchanged. To show that it is sufficient to demonstrate that $\{S_1, p_z\}$, $\{S_1, \mu\}$ and $\{S_1, \theta\}$ represent contributions of the next order with respect to the FLR decomposition. This demonstration is summarized into the Appendix.

For that reason, at the lowest FLR order the *gyrocenter* transformation can be interpreted as a simple shift of spatial coordinate with respect to the displacement $\boldsymbol{\rho}_1$.

Remark, that in the electrostatic case, it is easier to demonstrate that fact since the generating function of the *gyrocenter* transformation is given by the fluctuating part of the electrostatic potential $\phi_1 = \phi_1(\mathbf{X}+\boldsymbol{\rho}_0)$ and does not involve any p_z dependencies.

Since we still working in the p_z-representation, the expression for the Poisson Bracket remains unchanged under the FLR truncation. However, the expression for the second order $\sim \mathcal{O}(\epsilon_\delta^2)$ contributions to the reduced Hamiltonian will be affected.

Following the general procedure of the Hamiltonian transformation given by the Eq. (22), we consider:

$$e^{-\pounds_{S_1}} \psi_1(\mathbf{X} + \boldsymbol{\rho}_0) = \psi_1(\mathbf{X} + \boldsymbol{\rho}_0 + \boldsymbol{\rho}_1)$$

and therefore:

$$\psi_1(\mathbf{X} + \boldsymbol{\rho}_0 + \boldsymbol{\rho}_1) = \psi_1(\mathbf{X} + \boldsymbol{\rho}_0) + \boldsymbol{\rho}_1 \cdot \boldsymbol{\nabla} \psi_1(\mathbf{X} + \boldsymbol{\rho}_0) + \mathcal{O}(\epsilon_\delta^3),$$

now comparing this expression with formal Lie-transform implementation:

$$e^{-\pounds_{S_1}} \psi_1(\mathbf{X} + \boldsymbol{\rho}_0) = \psi_1(\mathbf{X} + \boldsymbol{\rho}_0) + \{S_1, \psi_1(\mathbf{X} + \boldsymbol{\rho}_0)\} + \mathcal{O}(\epsilon_\delta^3)$$

we identify that

$$\{S_1, \psi_1(\mathbf{X} + \boldsymbol{\rho}_0)\} = \boldsymbol{\rho}_1 \cdot \boldsymbol{\nabla} \psi_1(\mathbf{X} + \boldsymbol{\rho}_0). \tag{40}$$

Taking into the account the condition for definition of the generating function S_1 given by the Eq. (25) and the fact that $\mathcal{J}_0\left(\{S_1, \widetilde{\psi}_1\}\right) = \mathcal{J}_0\left(\{S_1, \psi_1\}\right)$, we recover the same partial cancellation of the second order terms as in the full FLR case given by the Eq. (29).

Finally, at the leading order in ρ_0 the second order electromagnetic contribution is:

$$\mathcal{J}_0\left(\left\{S_1, \widetilde{\psi}_1\left(\mathbf{X} + \boldsymbol{\rho}_0\right)\right\}\right) = -\mathcal{J}_0\left(\boldsymbol{\rho}_1 \cdot \boldsymbol{\nabla} \psi_1\right).$$

Therefore, using the above definition for $\boldsymbol{\rho}_1$ given by the Eq. (39), we find the same expression for the second order Hamiltonian as from the direct FLR series truncation of the full FLR model (33).

This demonstrates the link between the definition of the reduced particle position, and in particular the displacement $\boldsymbol{\rho}_1$, and the elimination of the gyrophase dependence of the reduced Hamiltonian dynamics.

6. Conclusions

In this work we have performed a detailed derivation of the second order gyrocenter Hamiltonian models in the case with full FLR corrections and within the *long-wavelength* approximation. The textitlong-wavelength model have been obtained in a two different ways: within the direct truncation of the full FLR model and by constructing the dynamical reduction procedure with the *gyrocenter* generating function, containing only the lowest order FLR contribution. We have explicitely shown that in the long-wavelength approximation, the gyrokinetic dynamical reduction resumes into the shift of the particle position, which clarifies the purpose of the complex gyrokinetic phase-space coordinate transformation.

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Appendix A. Velocity coordinate transformation

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