



A closed high-frequency Vlasov–Maxwell simulation model in toroidal geometry

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Abstract

A fully-kinetic ion and gyrokinetic electron Vlasov–Maxwell particle simulation model is derived through Lie transform perturbation theory for Hamiltonian systems in terms of four ordering parameters ϵ_B , ϵ_ω , $\epsilon_{||}$ and ϵ_δ . This model is closed by the field equations of Poisson's equation and Ampere' law. This scheme preserves the phase-space volume, and retains the ion cyclotron motion, while fine scale electron motion is ignored, so that the frequency falls in the range $\Omega_i \leq \omega < \Omega_e$. Using a perturbative method (δf), and ignoring the high order terms, this model is then formulated in a magnetic flux coordinate system with equilibrium Maxwellian distribution of particles. Thus, this model is especially suitable for the global particle simulation of high-frequency physical processes such as lower hybrid waves and waves in the ion cyclotron range of frequencies.

Keywords: fully-kinetic ion, gyrokinetic electron, radio frequency heating, lower hybrid wave, ion cyclotron range, particle simulation model, toroidal geometry

1. Introduction

Radio frequency (RF) waves have been proven to be an effective approach to plasma heating [1] and current drive [2] in magnetic confinement fusion plasmas, and are essential for the startup of a fusion reactor and its steady state operation thereafter. RF wave launching is also important to improve confinement, and to maintain H-mode runs of Tokamaks. However, the in-depth understanding on RF waves is still limited, especially in curvilinear coordinates with realistic equilibrium and profiles.

The application and investigation of RF waves can be traced back to the very beginning of magnetic confinement fusion research. Due to the stringent limitations to available computing resources, ray tracing simulations [3], which treat wave propagation in the eikonal form based on the Wentzel–Kramers–Brillouin (WKB) [4] approximation, were proposed

first, and have played an important role in the early days due to their simplicity. Ray tracing simulations can track the propagation of waves efficiently when wave–particle interactions or mode conversions can be ignored. Recently, by applying advanced wave solvers and Fokker–Planck collision solvers, global full wave codes, such as TORIC [5] and AORSA [6], can tackle the power deposition and mode conversion with a quasi-linear plasma response.

With the rapid development of super-computing, first-principles particle simulations [7] that directly solve kinetic equations are gradually emerging as a power tool for non-linear physical phenomena. Gyrokinetic (GK) simulations have long been successfully used to investigate low frequency plasma turbulence and transport in space and laboratory plasmas [8–10] through numerically evolving the gyro-phase-averaged Vlasov–Maxwell differential equation systems [11]; these have encompassed the code development of

massively parallelized fusion simulation codes over the last two decades, for both the particle in cell (PIC) method—such as GTC [8], GT3D [12], and GTS [13]—and continuum method—such as GYRO [14], GS2 [15], and GENE [16]. The massively parallel global gyrokinetic toroidal code (GTC), for example, has successfully incorporated the gyrokinetic electromagnetic field equations along with gyrokinetic [17], drift kinetic [18], fluid [19] and fluid-kinetic hybrid [20, 21] descriptions for different species of particles with distinct temporal-spatial characteristics in one single code. GTC has been first successfully applied to the investigation of electrostatic turbulence and transport problems, such as ion temperature gradient [22], electron temperature gradient [23] and trapped electron mode turbulence [24]. Pressure-driven electromagnetic Alfvén instabilities, such as TAE [25], BAE [26] and RSAE [27], and current-driven modes like kink and tearing modes have been studied by GTC as well.

Gyrokinetic theory for high frequency modes was first attempted by Chen Liu [28, 29] and later by Chiu [30]. A more general theory and computing technique for RF waves was proposed in 2000 by Hong Qin's G-gauge theory [31], which was used to develop a particle simulation code [32] to study high frequency waves in magnetized plasmas [33]. As a pioneering work in kinetic simulations of RF waves in toroidal geometry, GTC [34, 35] has been applied to investigate lower hybrid wave (LHW) physics using a simple and efficient scheme with fluid ion plus drift-kinetic electron in cylindrical and toroidal geometry [36] recently. Linear dispersion relations and nonlinear effects in ion Bernstein waves [37] were then verified using fully kinetic ions.

For high-frequency problems whose frequency is near or higher than the ion cyclotron frequency but lower than the electron cyclotron frequency, such as ion cyclotron range of frequencies (ICRF) waves and LHW, the gyromotion of ion species, denoted by subscript i , should be retained, whereas the fine scale gyromotion of electron species itself, denoted by subscript e , can be neglected due to clear temporal scale separation, while the coarse-grained finite Larmor radius (FLR) effect of electrons should be retained.

Based on Frieman–Chen nonlinear gyrokinetic theory [17], Yu Lin [38] first creatively proposes a gyrokinetic electron and fully-kinetic ion approach to deal with the plasma dynamics whose time scale ranges from Alfvén frequency to lower hybrid frequency. In that model, the gyrokinetic electron and fully-kinetic ion equations, Poisson's equation, Ampère's law and force balance equation are integrated to construct a closed simulation scheme, which is named GeFi [38, 39]. Instead of directly solving the perpendicular Ampère's law, GeFi applies the force balance equation to calculate the perturbed parallel magnetic field δB_{\parallel} , which is then used to compute the perturbed vector potential $\delta \mathbf{A}$ through Ampère's law. A two dimensional kinetic code based on this model was then developed in slab geometry to study the physics of Harris sheet [40] and tearing instability [41], which was followed by the simulations of propagation property [42] and Landau damping [43] of LHW in uniform plasmas.

A fully kinetic ion gyrokinetic/drift kinetic electron simulation model [44–46] was independently developed later, to

remove the limitations of gyrokinetic ions on simulations of turbulent transport. In that model, ions are treated by fully kinetic description and electrons are treated by gyrokinetic theory [45] or drift kinetic theory [46] when taking the long wavelength limit. Unlike GeFi, Faraday's equation and Ampère's law are used to close this simulation model.

In this work, the mature Lie-transform perturbation theory for Hamiltonian systems [47–51] is applied to construct a closed Vlasov–Maxwellian simulation model, utilizing the combination of gyrokinetic electrons and fully-kinetic ions [38, 39]. This model is useful for high-frequency physical processes, for example heating by RF waves such as ICRF waves, parametric decay instability of LHW, and lower hybrid current drive (LHCD). The Lie-transform gyrokinetic theory holds the natural conservation of energy and phase-space volume, as well as convenient higher-order nonlinear extensions. This Vlasov–Maxwell system is directly closed by Poisson's equation and Ampère's law, in contrast to the force-balance closure in GeFi [38, 39] and the closure using Faraday's equation in the Chen–Parker model [44–46]. We then rewrite the distribution equations with the low noise nonlinear characteristic δf form, and construct a closed system to solve the evolution of particles and perturbed electromagnetic field. Finally, we cast the Vlasov–Maxwell system into toroidal geometry by employing a magnetic flux coordinate system.

The following temporal-spatial ordering parameters ϵ_B , ϵ_F , ϵ_ω , ϵ_{\parallel} , and ϵ_δ are used to derive the nonlinear gyrokinetic equations for electrons. The background plasma is described by the small parameters ϵ_B and ϵ_F as

$$\frac{\rho_e}{L_B} \sim \epsilon_B \sim \frac{\rho_e}{L_F} \sim \epsilon_F,$$

where L_F and L_B are the characteristic lengths of the background distribution and magnetic field; $\rho_e = v_{te}/\Omega_e$ is the electron gyroradius, v_{te} is the electron thermal speed; $\Omega_e = (q_e B_0)/(m_e c)$ is the electron cyclotron frequency in unperturbed magnetic field B_0 ; q_e and m_e are the charge and mass of electrons, respectively. The temporal ordering of fluctuating fields is

$$\frac{\omega}{\Omega_e} \sim \epsilon_\omega$$

where ω is the characteristic frequency of fluctuations. There are various mechanisms of wave-particle interaction, ranging from Alfvén frequency to lower hybrid frequency, such as the ion Landau damping, ion cyclotron resonance damping, and electron Landau damping. Unlike the relationship between parallel wave number k_{\parallel} and perpendicular wave number k_{\perp} in ion gyrokinetic theory, a small parameter ϵ_{\parallel} has been used to describe the spatial ordering

$$k_{\perp} \rho_e \equiv \epsilon_{\perp} \quad \text{and} \quad k_{\parallel} \rho_e \sim \epsilon_{\parallel} \ll 1,$$

where $\epsilon_{\perp} \gg \epsilon_{\parallel}$. The amplitude of perturbed field is described by the small parameter ϵ_δ ,

$$\frac{\delta B}{B} \sim \frac{\delta f}{f} \sim \frac{q \delta \phi}{T_e} \sim \epsilon_\delta,$$

where δB is the amplitude of perturbed magnetic field, δf is the perturbed distribution function, and $\delta\phi$ is the perturbed electrostatic potential. The relationships of these parameters are different for various physical processes. Although they are treated approximately equally during the model derivation, i.e., $\epsilon_\omega \sim \epsilon_\parallel \sim \epsilon_B \sim \epsilon_\delta \sim \epsilon$, their natures are still retained. In addition, these small parameters that appear ahead of physical quantities in the rest of this paper act as indexes that indicate the ordering of these quantities.

The outline of this paper is as follows. In section 2, the fully kinetic equation for ions is given, and the gyrokinetic equations are derived with Lie transform perturbation theory for Hamiltonian systems. In section 3, moments of distribution are obtained for ion and electron species, respectively. In section 4, the gyrokinetic Maxwell's equations are derived in terms of moments. In section 5, another form of Ampère's law is elucidated. In section 6, the total energy of system is proven to be invariant. In section 7, the weight evolution equations of particles are shown and a closed system is constructed. In section 8, we introduce the magnetic flux coordinate system and formulate this model in Tokamak geometry. In section 9, a discussion is given. Conclusions are presented in section 10.

2. Particle dynamics

In this section, the momentum equations and distribution functions for fully-kinetic ion species and gyrokinetic electron species are derived through Hamiltonian equations. In the first part of this section, the dynamics of fully kinetic ions are developed using single particle Hamiltonian theory in canonical phase space, so that the ion cyclotron damping is retained. In the second part, as our target frequency range is much lower than the electron cyclotron frequency, the dynamics of electrons can be described by gyrokinetic theory that is developed using gyrocenter Hamiltonian theory [51] with the electron FLR effect retained. By dropping the gyro-angle component that describes the electrons' fast gyromotion, the electrons' single-particle Hamiltonian is transformed from the particles' six-dimensional phase space to the five-dimensional gyrocenter phase space where the magnetic moment is an adiabatic invariant in the Lie-transform perturbation method.

2.1. Fully-kinetic ion

In order to preserve the phase-space volume, a Hamiltonian system [52, 53] is constructed using a set of canonical coordinates (x^α, p_α) . In the canonical phase space, the canonical Poisson bracket can be defined in terms of two arbitrary phase-space functions F and G

$$\{F, G\} = \frac{\partial F}{\partial x^\alpha} \frac{\partial G}{\partial p_\alpha} - \frac{\partial F}{\partial p_\alpha} \frac{\partial G}{\partial x^\alpha},$$

where x^α is the ion's position, $p_\alpha = m_i \dot{x}^\beta g_{\alpha\beta} + q_i A_\alpha / c$ is the ion's canonical momentum, m_i is the ion mass, q_i is the ion charge, $\dot{x}^\beta = (dx^\beta) / (dt)$ is the time derivative of x^β , $g_{\alpha\beta}$ is the component of the gauge tensor in configuration

space as given in appendix, and the total vector potential $A_\alpha = A_{0\alpha} + \epsilon_\delta \delta A_\alpha$ consists of the equilibrium part $A_{0\alpha}$ and the perturbed part δA_α . In an electromagnetic field, the canonical phase-space Hamiltonian $H_i(x^\alpha, p_\alpha, t)$ of an ion can be written as

$$H_i = \frac{1}{2m_i} \left[\left(p_\alpha - \frac{q_i}{c} A_\alpha \right) \left(p_\beta - \frac{q_i}{c} A_\beta \right) g^{\alpha\beta} \right] + q_i \phi,$$

where the total electrostatic potential $\phi = \phi_0 + \epsilon_\delta \delta\phi$ is expressed in terms of the equilibrium part ϕ_0 and the perturbed part $\delta\phi$. For simplicity, the Hamilton's equations in the absence of ϕ_0 are derived afterwards,

$$\begin{aligned} \dot{x}^\alpha &= \{x^\alpha, H_i\} = \frac{1}{m_i} \left(p^\alpha - \frac{q_i}{c} A^\alpha \right), \\ \dot{p}_\alpha &= \{p_\alpha, H_i\} = -\frac{1}{2m_i} \left(p_\beta p_\gamma \frac{\partial g^{\beta\gamma}}{\partial x^\alpha} - \frac{2q_i}{c} p_\beta \frac{\partial A^\beta}{\partial x^\alpha} + \frac{q_i^2}{c^2} \frac{\partial A^2}{\partial x^\alpha} \right) \\ &\quad - q_i \epsilon_\delta \frac{\partial \delta\phi}{\partial x^\alpha}. \end{aligned}$$

The Vlasov equation in the canonical phase space is given by

$$\frac{df_i}{dt} = \frac{\partial f_i}{\partial t} + \{f_i, H_i\} = \frac{\partial f_i}{\partial t} + \dot{x}^\alpha \frac{\partial f_i}{\partial x^\alpha} + \dot{p}_\alpha \frac{\partial f_i}{\partial p_\alpha} = 0, \quad (1)$$

where f_i is the ion distribution function in the canonical phase space.

2.2. Gyrokinetic electron

In modern nonlinear gyrokinetic theory [51] based on the Lie-transform perturbation method [54–56], there are usually two steps to reduce the dynamics of single particle Hamiltonian systems to decouple the fast gyromotion from the slow-varying gyrocenter motion and electromagnetic field. Firstly, the Hamiltonian system is transformed from unperturbed extended particle phase space $z(\mathbf{x}, p_{e\parallel 0}, \mu_0, \Theta_0, w, t)$ to guiding-center phase space $\mathcal{Z}(\mathbf{X}, p_{e\parallel}, \mu, \Theta, w, t)$, where \mathbf{x} is the particle position, $\mu_0 = mv_{e\perp}^2 / (2B_0)$ is the magnetic moment in particle phase space, Θ_0 is the phase angle, $p_{e\parallel 0} = mv_{e\parallel}$ is the kinetic momentum parallel to the equilibrium magnetic field, and (w, t) are the canonically conjugate guiding-center energy and time coordinates, respectively. The first step makes the guiding-center phase angle Θ an ignorable coordinate by design and the magnetic moment μ an adiabatic invariant. Secondly, the Hamiltonian system is transformed from guiding-center phase space $\mathcal{Z}(\mathbf{X}, p_{e\parallel}, \mu, \Theta, w, t)$ to gyrocenter phase space $\bar{\mathcal{Z}}(\bar{\mathbf{X}}, \bar{p}_{e\parallel}, \bar{\mu}, \bar{\Theta}, \bar{w}, t)$ in the presence of the electromagnetic fluctuations that destroy the symmetry of the guiding-center Hamiltonian system. In this second step, the dynamic system attains a new symmetry by introducing a gyrocenter phase angle $\bar{\Theta}$, which is again an ignorable component, and a new adiabatic-invariant magnetic moment $\bar{\mu}$. In this work, the Hamiltonian gyrokinetic model is chosen, and the gyrocenter parallel momentum is thus the canonical momentum [57].

In this work, by following the usual derivation procedure, the gyrokinetic equations are built upon Lie-transform perturbation theory for Hamiltonian systems. Given the Hamiltonian gyrokinetic model, the unperturbed and perturbed Hamiltonian in the extended gyrocenter phase space are

$$\bar{\mathcal{H}}_{0\text{gy}} = \bar{H}_{0\text{gy}} - \bar{w} = \frac{\bar{p}_{e\parallel}^2}{2m_e} + \bar{\mu}B_0 - \bar{w},$$

$$\bar{H}_{1\text{gy}} = \epsilon_\delta q_e \langle \delta\phi_{\text{gc}}^* \rangle,$$

and accordingly, the Poisson bracket in the extended gyrocenter phase space is defined in terms of two arbitrary functions \mathcal{F} and \mathcal{G}

$$\{\mathcal{F}, \mathcal{G}\} = \frac{q_e}{m_e c} \left(\frac{\partial \mathcal{F}}{\partial \bar{\Theta}} \frac{\partial \mathcal{G}}{\partial \bar{\mu}} - \frac{\partial \mathcal{F}}{\partial \bar{\mu}} \frac{\partial \mathcal{G}}{\partial \bar{\Theta}} \right) + \frac{\mathbf{B}_0^*}{B_{\parallel}^*} \cdot \left(\bar{\nabla} \mathcal{F} \frac{\partial \mathcal{G}}{\partial \bar{p}_{e\parallel}} - \frac{\partial \mathcal{F}}{\partial \bar{p}_{e\parallel}} \bar{\nabla} \mathcal{G} \right) - \frac{c\hat{\mathbf{b}}}{q_e B_{\parallel}^*} \cdot \bar{\nabla} \mathcal{F} \times \bar{\nabla} \mathcal{G} + \left(\frac{\partial \mathcal{F}}{\partial \bar{w}} \frac{\partial \mathcal{G}}{\partial t} - \frac{\partial \mathcal{F}}{\partial t} \frac{\partial \mathcal{G}}{\partial \bar{w}} \right),$$

where the modified magnetic field is

$$\mathbf{B}_0^* = \mathbf{B}_0 + \epsilon_B \frac{B_0 p_{e\parallel}}{m_e \Omega_e} \nabla \times \hat{\mathbf{b}}, \quad (2)$$

$B_{\parallel}^* = \hat{\mathbf{b}} \cdot \mathbf{B}_0^*$, and $\hat{\mathbf{b}}$ is the unit basis vector parallel to the unperturbed magnetic field \mathbf{B}_0 . The effective potential

$$\delta\phi_{\text{gc}}^* = \delta\phi_{\text{gc}} - \frac{\delta \mathbf{A}_{\text{gc}}}{c} \cdot \left(\frac{p_{e\parallel}}{m_e} \hat{\mathbf{b}} + \Omega_e \frac{\partial \rho_{\text{gc}}}{\partial \bar{\Theta}} \right),$$

includes perturbed scalar potential $\delta\phi_{\text{gc}}(\mathbf{X}, t)$ and vector potential $\delta \mathbf{A}_{\text{gc}}(\mathbf{X}, t)$ in the guiding-center phase space, where $\rho_{\text{gc}} = (2\mu B_0/m_e)^{1/2} \hat{\rho}/\Omega_e$ is the guiding-center gyroradius derived from the guiding-center phase-space transformation [51, 58], and $\hat{\rho}$ is the unit vector in the direction of ρ_{gc} .

The gyrokinetic Vlasov equation for electrons in six-dimensional gyrocenter phase space $(\bar{\mathbf{X}}, \bar{p}_{e\parallel}, \bar{\mu}, \bar{\Theta})$ is expressed by

$$\frac{\partial \bar{F}_e}{\partial t} + \dot{\bar{\mathbf{X}}} \cdot \frac{\partial \bar{F}_e}{\partial \bar{\mathbf{X}}} + \dot{\bar{p}}_{e\parallel} \frac{\partial \bar{F}_e}{\partial \bar{p}_{e\parallel}} = 0, \quad (3)$$

in terms of the Hamilton's equations

$$\dot{\bar{p}}_{e\parallel} = -\frac{\epsilon_{\parallel} \epsilon_\delta}{\epsilon_B} q_e \frac{\mathbf{b}^*}{b_{\parallel}^*} \cdot \bar{\nabla} \langle \delta\phi_{\text{gc}}^* \rangle - \bar{\mu} \frac{\mathbf{b}^*}{b_{\parallel}^*} \cdot \bar{\nabla} B_0, \quad (4)$$

$$\dot{\bar{\mathbf{X}}} = \left(\frac{\bar{p}_{e\parallel}}{m_e} + \epsilon_\delta \frac{\partial \langle \delta\phi_{\text{gc}}^* \rangle}{\partial \bar{p}_{e\parallel}} \right) \frac{\mathbf{b}^*}{b_{\parallel}^*} + \frac{c}{q_e B_{\parallel}^*} \hat{\mathbf{b}} \times [\epsilon_\delta q_e \bar{\nabla} \langle \delta\phi_{\text{gc}}^* \rangle + \epsilon_B \bar{\mu} \bar{\nabla} B_0], \quad (5)$$

where $\bar{F}_e(\bar{\mathbf{X}}, \bar{p}_{e\parallel}, \bar{\mu})$ is the gyrocenter distribution function of electrons, $\mathbf{b}^* = \hat{\mathbf{b}} + \epsilon_B \bar{p}_{e\parallel} / (m_e \Omega_e) \bar{\nabla} \times \hat{\mathbf{b}}$ and $b_{\parallel}^* = \hat{\mathbf{b}} \cdot \mathbf{b}^*$.

3. Distribution moments

A closed self-consistent description of the interactions involving the perturbed electromagnetic fields and Vlasov

distribution implies that the Maxwell equations can be written with moments expressed by the distribution function.

3.1. Moments of ion species

Since the ion distribution evolves in particle phase space, the moments of ion distribution can be directly derived from the distribution function in particle phase space immediately

$$n_i = \int f_i d^3 p_i,$$

$$\mathbf{J}_i = \int \mathbf{v}_i f_i d^3 p_i,$$

$$\mathbf{P}_i = \int \mathbf{v}_i \mathbf{v}_i f_i d^3 p_i,$$

where f_i is the distribution of ion species, and equilibrium distribution is set to be Maxwellian.

3.2. Moments of electron species in the pull-back representation

The electron distribution is transformed from gyrocenter phase space to particle phase space in order to conform with the ion phase-space. The distribution function of electrons takes different forms in gyrocenter phase space with GK approximation and in guiding-center phase space with drift-kinetic approximation. The particle phase-space, guiding-center and gyrocenter distribution is connected through the phase-space transformations. The unperturbed distribution function of electrons in five-dimensional gyrocenter phase space can be written as a local Maxwellian equation in the thermal equilibrium form

$$\bar{F}_{e0}(\bar{\mathcal{Z}}) = \bar{N}_{e0} \left(\frac{m_e}{2\pi \bar{T}_e} \right)^{3/2} \exp\left(-\frac{E_e}{\bar{T}_e}\right), \quad (6)$$

where $E_e = \bar{\mu}B_0 + \bar{p}_{e\parallel}^2/2m_e$ is the unperturbed gyrocenter Hamiltonian $\bar{H}_{0\text{gy}}$.

In Hamiltonian gyrokinetic model, the first order gyrocenter generating vector field [51, 59]

$$G_1^a = \{S_1, \mathcal{Z}^a\} + \epsilon_\delta \frac{q_e}{c} \delta \mathbf{A}_{\text{gc}} \cdot \{\mathbf{X} + \epsilon_B \rho_{\text{gc}}, \mathcal{Z}^a\},$$

is derived via the transformation of the symplectic form of gyrocenter phase-space Lagrangian, where the first order gauge scalar field $S_1 = q_e \int (\delta\phi_{\text{gc}}^* - \langle \delta\phi_{\text{gc}}^* \rangle) d\bar{\theta}/\Omega_e$ is chosen to ensure that the perturbed gyrocenter Hamiltonian $\bar{H}_{1\text{gy}}$ is independent of gyrocenter gyro-angle $\bar{\Theta}$. Based on the Lie-transform perturbation theory for Hamiltonian systems, the guiding-center distribution function F_e can be yielded by applying pull-back transformation $T_{\text{gy}} = 1 + \epsilon_\delta G_1^a \partial/\partial \mathcal{Z}^a$ to gyrocenter distribution function \bar{F}_e ,

$$\begin{aligned} F_e(\mathcal{Z}) &= \bar{F}_e(T_{\text{gy}}\mathcal{Z}) = \bar{F}_e(\mathcal{Z}) + \epsilon_\delta G_1^a \frac{\partial \bar{F}_e(\mathcal{Z})}{\partial \mathcal{Z}^a} \\ &= \bar{F}_e(\mathcal{Z}) + \epsilon_\delta \{S_1, \bar{F}_{e0}\} + \epsilon_\delta \frac{q_e}{c} \delta \mathbf{A}_{\text{gc}} \cdot \{\mathbf{X} + \epsilon_B \rho_{\text{gc}}, \bar{F}_{e0}\} \\ &= \bar{F}_e - \epsilon_\delta \frac{q_e \bar{F}_{e0}}{\bar{T}_e} [\delta\phi_{\text{gc}} - \langle \delta\phi_{\text{gc}}^* \rangle], \end{aligned}$$

where $G_1^a \partial \bar{F}_{e1} / \partial Z^a$ comprises higher order terms and has been neglected. According to the first order vector generating field of guiding-center transformation as appendix B in Ref. 46, at the lower order, the pull-back transformation T_{gc} from guiding-center distribution function F_e to particle-space distribution function f_e gives

$$\begin{aligned} f_e(z) = F_e(T_{gc}z) &= \frac{(1 - \epsilon_B \rho_e \cdot \nabla) \bar{N}_{e0} [m_e / (2\pi)]^{3/2}}{[(1 - \epsilon_B \rho_e \cdot \nabla) \bar{T}_e]^{3/2}} \\ &\times \exp \left[-\frac{\mu_0 B_0 + p_{e\parallel 0}^2 / 2m_e}{(1 - \epsilon_B \rho_e \cdot \nabla) \bar{T}_e} \right] + \epsilon_\delta \delta \bar{F}_e \\ &- \epsilon_\delta \rho_e \cdot \nabla \delta F_e - \epsilon_\delta \frac{(1 - \epsilon_B \rho_e \cdot \nabla) q_e \bar{N}_{e0} [m_e / (2\pi)]^{3/2}}{[(1 - \epsilon_B \rho_e \cdot \nabla) \bar{T}_e]^{5/2}} \\ &\times \exp \left[-\frac{\mu_0 B_0 + p_{e\parallel 0}^2 / 2m_e}{(1 - \epsilon_B \rho_e \cdot \nabla) \bar{T}_e} \right] \\ &\times \left[\delta \phi - J_0 \exp(\rho_e \cdot \nabla) \delta \phi + J_0 \frac{p_{e\parallel 0}}{cm_e} \exp(\rho_e \cdot \nabla) \delta A_{\parallel} \right. \\ &\left. + \frac{1}{c} \sqrt{\frac{2\mu_0 B_0}{m_e}} \exp(\rho_e \cdot \nabla) \left(iJ_1 \frac{\mathbf{k}_\perp \times \hat{\mathbf{b}}}{k_\perp} \cdot \delta \mathbf{A}_\perp \right) \right], \end{aligned}$$

where J_n is the n th-order Bessel function, and $\rho_e = (2\mu_0 B_0 / m_e)^{1/2} \hat{\rho}_0 / \Omega_e$ is the particle-space gyroradius. Since for lower hybrid wave and ICRF waves, the wavelength is commonly larger than the electron gyroradius, the long wavelength approximation is reasonable, i.e. $k_\perp \rho_e < 1$.

Electron number density is given by the zeroth moment of distribution function

$$\begin{aligned} n_e(\mathbf{r}) &= \int f_e(z) \delta(\mathbf{x} - \mathbf{r}) d\mathbf{x} d\mathbf{v} = \int \bar{F}_e(T_e z) d^3 p_e \\ &= \bar{N}_{e0} + \epsilon_\delta \delta \bar{N}_e + \epsilon_\delta \left[\frac{c \bar{N}_{e0}}{B_0 \Omega_e} \nabla_\perp^2 \delta \phi + \frac{\bar{N}_{e0}}{B_0} \nabla \cdot (\delta \mathbf{A} \times \hat{\mathbf{b}}) \right], \end{aligned} \quad (7)$$

where $T_e z = T_{gc} T_{gy} z$, $\bar{N}_{e0} = \int \bar{F}_{e0} d^3 p_e$ is the unperturbed gyrocenter electron number density, $\delta \bar{N}_e = \int \delta \bar{F}_e d^3 p_e$ is the perturbed gyrocenter electron number density, and $\int d^3 p_e = \int B_0 / m_e^2 d\mu_0 dp_{e\parallel} d\Theta_0$ denotes an integration over the particle momentum space, since the gyrocenter phase-space distribution has been transformed into particle phase space.

The first moment is the electron current

$$\begin{aligned} \mathbf{J}_e(\mathbf{r}) &= \int q_e \mathbf{v}_e f_e(z) \delta(\mathbf{x} - \mathbf{r}) d\mathbf{x} d\mathbf{v} = \epsilon_\delta \delta \bar{\mathbf{J}}_e - \epsilon_\delta \frac{\bar{N}_{e0} q_e^2}{cm_e} \delta A_{\parallel} \hat{\mathbf{b}} \\ &+ \epsilon_\delta \frac{c q_e \bar{N}_{e0}}{B_0} \hat{\mathbf{b}} \times \nabla \delta \phi + \epsilon_\delta \frac{3c^2 \bar{N}_{e0} \bar{T}_e}{2B_0^2 \Omega_e} \hat{\mathbf{b}} \times \nabla_\perp \nabla_\perp^2 \delta \phi \\ &+ \epsilon_\delta \frac{2c \bar{N}_{e0} \bar{T}_e}{B_0^2} \hat{\mathbf{b}} \times \nabla \left[\nabla \cdot (\delta \mathbf{A} \times \hat{\mathbf{b}}) \right] + \epsilon_B \frac{\hat{\mathbf{b}}}{B_0} \times \nabla (c \bar{N}_{e0} \bar{T}_e), \end{aligned} \quad (8)$$

where

$$\delta \bar{\mathbf{J}}_e = \hat{\mathbf{b}} \int q_e \frac{p_{e\parallel 0}}{m_e} \delta \bar{F}_e d^3 p_e + \hat{\mathbf{b}} \times \nabla \int c \mu_0 \delta \bar{F}_e d^3 p_e.$$

The second moment gives the pressure tensor of electrons

$$\begin{aligned} \mathbf{P}_e(\mathbf{r}) &= \int m_e \mathbf{v}_e \mathbf{v}_e f_e(z) \delta(\mathbf{x} - \mathbf{r}) d\mathbf{x} d\mathbf{v} \\ &= \bar{N}_{e0} \bar{T}_e \mathbf{I} + \epsilon_\delta \delta \bar{\mathbf{P}}_e + \epsilon_\delta \frac{\bar{N}_{e0} \bar{T}_e}{B_0} \left[2\delta B_{\parallel} \left(\mathbf{I} - \frac{1}{2} \hat{\mathbf{b}} \hat{\mathbf{b}} \right) \right. \\ &+ \frac{3}{2} \frac{c}{\Omega_e} \nabla_\perp^2 \delta \phi \left(\mathbf{I} - \hat{\mathbf{b}} \hat{\mathbf{b}} \right) + \delta \mathbf{B}_\perp \hat{\mathbf{b}} + \hat{\mathbf{b}} \delta \mathbf{B}_\perp \\ &\left. + \frac{c}{\Omega_e} \nabla_\perp^2 \delta \phi \hat{\mathbf{b}} \hat{\mathbf{b}} + \frac{c}{\Omega_e} (\mathbf{b} \times \nabla) (\mathbf{b} \times \nabla) \delta \phi \right], \end{aligned}$$

where

$$\delta \bar{\mathbf{P}}_e = \int \left[\frac{p_{e\parallel 0}^2}{m_e} \hat{\mathbf{b}} \hat{\mathbf{b}} + \mu_0 B_0 \left(\mathbf{I} - \hat{\mathbf{b}} \hat{\mathbf{b}} \right) \right] \delta \bar{F}_e d^3 p_e.$$

4. Gyrokinetic Maxwell's equations

The perpendicular and parallel wave-number satisfies the ordering $k_\perp \gg k_\parallel$, which implies that $\nabla^2 \delta \phi$ can be reduced to $\nabla_\perp^2 \delta \phi$, and the undesired high frequency Langmuir oscillation along the unperturbed magnetic field is suppressed naturally. This reduction results in the generalized Poisson's equation

$$\begin{aligned} \left(1 + \sum_e \frac{\omega_{pe}^2}{\Omega_e^2} \right) \nabla_\perp^2 \delta \phi + \sum_e \frac{4\pi q_e \bar{N}_{e0}}{B_0} \nabla \cdot (\delta \mathbf{A} \times \hat{\mathbf{b}}) \\ = -4\pi \left(\sum_i q_i \delta n_i + \sum_e q_e \delta \bar{N}_e \right), \end{aligned} \quad (9)$$

where $\delta n_i = \int \delta f_i d^3 p_i$ is the perturbed ion number density, \sum_i and \sum_e denote the summation over all the ion and electron species, $\omega_{pe} = 4\pi \bar{N}_{e0} q_e^2 / m_e$ is the electron plasma frequency, and the quasi-neutrality condition $\sum_i q_i \bar{n}_{i0} + \sum_e q_e \bar{N}_{e0} = 0$ has been used. The second and third polarization terms on the left-hand side of equation (9) come from the drift of electron gyrocenter under the perturbed electromagnetic fluctuations (7). The Maxwell equations are on the order of ϵ_δ , which is left out for conciseness wherever it can be canceled out on both sides in sections 4 and 5.

Providing Coulomb gauge $\nabla \cdot \mathbf{A} = 0$ is satisfied, the gyrokinetic Ampère's law reads

$$-\nabla_\perp^2 \delta \mathbf{A} = \frac{4\pi}{c} (\delta \mathbf{J}_i + \delta \mathbf{J}_e).$$

With the electron current (8), Ampère's law becomes

$$\begin{aligned} -\nabla_\perp^2 \delta \mathbf{A} - \sum_e \beta_{e0} \nabla_\perp^2 \delta \mathbf{A}_\perp + \sum_i \frac{\omega_{pi}^2}{c^2} \delta \mathbf{A} + \sum_e \frac{\omega_{pe}^2}{c^2} (\delta \mathbf{A} \cdot \hat{\mathbf{b}}) \hat{\mathbf{b}} \\ - \sum_e \left[\frac{4\pi q_e \bar{N}_{e0}}{B_0} \hat{\mathbf{b}} \times \nabla \delta \phi + \frac{6\pi c \bar{P}_{e0}}{B_0^2 \Omega_e} \hat{\mathbf{b}} \times \nabla_\perp \nabla_\perp^2 \delta \phi \right] \\ = \frac{4\pi}{c} \left(\sum_i \delta \mathbf{J}_i + \sum_e \delta \bar{\mathbf{J}}_e \right), \end{aligned} \quad (10)$$

where $\beta_{e0} = 8\pi\bar{N}_{e0}\bar{T}_e/B_0^2$ is the ratio of kinetic to magnetic energy densities, $\omega_{pi} = 4\pi n_{i0}q_i^2/m_i$ is the ion plasma frequency, and $\bar{P}_{e0} = \bar{N}_{e0}\bar{T}_e$ is the electron equilibrium thermal pressure. When the perpendicular wavelength is longer than electron collisionless skin depth c/ω_{pe} , equation (10) is difficult to solve, because the fourth term on the left-hand side and the parallel component of the second term on the right-hand side dominate and nearly cancel each other [60, 61]. This is a challenge for low frequency Alfvén waves. However, for LHW and ICRF waves, the perpendicular wave length has the same order of magnitude as the electron skin depth, and the parallel wavelength is on the order of the ion skin depth c/ω_{pi} [35] from experimental parameters. Therefore, the canceling problem can be overcome.

5. Comparison with GeFi model

In the previous section, an efficient compact Vlasov–Maxwell system is constructed directly using Poisson’s equation and Ampère’s law in terms of scalar potential $\delta\phi$ and vector potential $\delta\mathbf{A}$. In order to compare with GeFi [38] model, the Vlasov–Maxwell system has to be closed by an alternative approach: the gyrokinetic Poisson’s equation and Ampère’s law is solved with the help of δB_{\parallel} as an intermediate variable in a non-symmetric way by decomposing Ampère’s law into components parallel and perpendicular to $\hat{\mathbf{b}}$. By plugging in the electron current (8), the parallel component of Ampère’s law reads

$$\begin{aligned} & -\nabla_{\perp}^2 \delta A_{\parallel} + \left(\sum_i \frac{\omega_{pi}^2}{c^2} + \sum_e \frac{\omega_{pe}^2}{c^2} \right) \delta A_{\parallel} \\ & = \frac{4\pi}{c} \left[\sum_e \int \frac{q_e P_{e\parallel 0}}{m_e} \delta \bar{F}_e d^3 p_e + \sum_i \left(\int \frac{q_i \mathbf{P}_i}{m_i} \delta f_i d\mathbf{p}_i \right) \cdot \hat{\mathbf{b}} \right], \end{aligned} \quad (11)$$

which is the same equation as equation (10) in the parallel direction, and the rewritten perpendicular component

$$\frac{c}{4\pi} \nabla \times (\delta B_{\parallel} \hat{\mathbf{b}}) = \delta \mathbf{J}_{i\perp} + \delta \mathbf{J}_{e\perp}$$

yields the ‘so-called pressure balance equation’ [59] of electrons

$$\begin{aligned} & -\sum_e q_e \bar{N}_{e0} \nabla_{\perp} \delta\phi = \nabla_{\perp} \left[\frac{1}{4\pi} \left(1 + \sum_e \beta_{e0} \right) B_0 \delta B_{\parallel} \right] + \sum_e \nabla_{\perp} \delta \bar{P}_{e\perp} \\ & + \left(\sum_i \delta \mathbf{J}_i \times \frac{\mathbf{B}_0}{c} \right) + \sum_e \nabla_{\perp} \left(\frac{3c\bar{P}_{e0}}{2B_0\Omega_e} \nabla_{\perp}^2 \delta\phi \right), \end{aligned} \quad (12)$$

where $\delta \bar{P}_{e\perp} = \int \mu_0 B_0 \delta \bar{F}_e d^3 p_e$ is the perpendicular component of $\delta \bar{\mathbf{P}}_e$. In this way, $\delta\phi$, δB_{\parallel} and δA_{\parallel} can be computed

by a set of scalar equations including equation (11), (12) and Poisson’s equation (9) in terms of δB_{\parallel}

$$\left(1 + \sum_e \frac{\omega_{pe}^2}{\Omega_e^2} \right) \nabla_{\perp}^2 \delta\phi + \sum_e \frac{4\pi q_e \bar{N}_{e0}}{B_0} \delta B_{\parallel} = -4\pi \left(\sum_i q_i \delta n_i + \sum_e q_e \delta \bar{N}_e \right).$$

$\delta \mathbf{A}_{\perp}$ is then computed by δB_{\parallel} through

$$\nabla \times \delta \mathbf{A}_{\perp} = \delta B_{\parallel} \hat{\mathbf{b}}.$$

At low order, the pressure balance equation derived from perpendicular Ampère’s law maintains the same form as GeFi’s force-balance equation. However, the pressure-balance equation is quantitatively different from the counterpart of GeFi, in that the coefficient of $c\bar{P}_{e0}\nabla_{\perp}^2\delta\phi/(B_0\Omega_e)$ is 3/2 in equation (12) in contrast to 1 in the GeFi model.

When ions evolve in canonical phase space, this approach is made relatively complicated by the introduction of the intermediate variable δB_{\parallel} , which is not used elsewhere, to solve the field equations. Therefore, the direct solution of Poisson’s equation and Ampère’s law listed in the previous section will be used in the rest of this article.

6. Energy conservation

The energy conservation of a global system usually serves as a significant test for a simulation model [62]. The property of conservation is the nature of Lie transform Hamilton theory. The nonlinear gyrokinetic energy conservation laws has been proven by prior works [47, 49, 59, 63, 64]. The total energy of system includes the particle kinetic energy and electromagnetic field energy

$$\begin{aligned} \mathcal{E} & = \sum_i \int H_{ik} f_i d^3 p_i d^3 x + \sum_e \int H_{ek} f_e d^3 v_e d^3 x \\ & + \frac{1}{8\pi} \int (\mathbf{E}^2 + \mathbf{B}^2) d^3 x, \end{aligned} \quad (13)$$

where

$$H_{ik} = \frac{(\mathbf{P}_i - q_i \mathbf{A}/c)^2}{2m_i}, \quad H_{ek} = \frac{1}{2} m_e v_e^2,$$

are the kinetic energy of ions and electrons respectively. The time derivative of \mathcal{E} is

$$\begin{aligned} \frac{d\mathcal{E}}{dt} & = \sum_i \frac{\partial}{\partial t} \int f_i H_{ik} d^3 p_i d^3 x + \sum_e \frac{\partial}{\partial t} \int H_{ek} f_e d^3 v_e d^3 x \\ & - \frac{1}{4\pi} \int \left[\delta\phi \frac{\partial}{\partial t} (\nabla^2 \delta\phi) - \frac{\partial \mathbf{A}}{\partial t} \cdot (\nabla \times \nabla \times \mathbf{A}) \right] d^3 x. \end{aligned}$$

By combining with Vlasov equations (1) and (3) and Maxwell equations (9) and (10), $d\mathcal{E}/dt$ [65] can be further reduced to

$$\begin{aligned}
\frac{d\mathcal{E}}{dt} &= \sum_i \int H_{ik} \frac{\partial f_i}{\partial t} d^3 p_i d^3 x + \sum_i \int f_i \frac{\partial H_{ik}}{\partial t} d^3 p_i d^3 x \\
&+ \sum_e \frac{\partial}{\partial t} \int H_e f_e d^3 v_e d^3 x \\
&+ \int \left[\delta \phi \frac{\partial}{\partial t} \left(\sum_i \int q_i f_i d^3 p_i + \sum_e \int q_e \int f_e d^3 v_e \right) \right. \\
&+ \left. \frac{\partial \mathbf{A}}{\partial t} \cdot \left(\sum_i \frac{q_i}{c} \int (\mathbf{p}_i - \mathbf{A}) f_i d^3 v_i + \sum_e \frac{q_e}{c} \int \mathbf{v}_e f_e d^3 v_e \right) \right] d^3 x \\
&= \sum_i \int H_i \frac{\partial f_i}{\partial t} d^3 p_i d^3 x - \sum_i \frac{q_i}{c} \int f_i (\mathbf{p}_i - \mathbf{A}) \cdot \frac{\partial \mathbf{A}}{\partial t} d^3 p_i d^3 x \\
&+ \sum_i \frac{q_i}{c} \int \frac{\partial \mathbf{A}}{\partial t} \cdot (\mathbf{p}_i - \mathbf{A}) f_i d^3 p_i d^3 x \\
&+ \sum_e \frac{\partial}{\partial t} \int \left(\bar{H}_{0gy} - \{S_1, \bar{H}_{0gy}\} - \frac{q_e}{c} \delta \mathbf{A}_{gc} \right. \\
&\cdot \left. \{ \mathbf{X} + \epsilon_B \rho_{gc}, \bar{H}_{0gy} \} \right) \bar{F}_e d^3 \bar{p}_e d^3 \bar{X} \\
&+ \sum_e q_e \int \left(\langle \delta \phi_{gc} \rangle \frac{\partial}{\partial t} F_e + \frac{1}{c} \left\langle \frac{\partial \delta \mathbf{A}_{gc}}{\partial t} \right. \right. \\
&\cdot \left. \left. \{ \mathbf{X} + \epsilon_B \rho_{gc}, \bar{H}_{0gy} \} \right\rangle \bar{F}_e \right) d^3 \bar{p}_e d^3 \bar{X} \\
&= - \sum_i \int \{ f_i H_i, H_i \} d^3 p_i d^3 x - \sum_e \int \{ \bar{F}_e \bar{H}_e, \bar{H}_e \} d\bar{p}_e d^3 \bar{X} \\
&= 0,
\end{aligned}$$

where

$$\bar{H}_e = \bar{H}_{0gy} + q_e \langle \delta \phi_{gc}^* \rangle,$$

and $\int d^3 \bar{p}_e d^3 \bar{X} = \int B_{\parallel}^* / m_e^2 d\bar{\mu} d\bar{p}_{e\parallel} d\bar{\Theta} d^3 \bar{X}$ denotes an integration over the gyrocenter phase space. Thus, the total energy of the system is invariant.

7. Perturbative scheme

The Vlasov equation can be linearized through decomposing quantities into unperturbed part with a subscript 0, and perturbed part with a prefix δ ,

$$\frac{\partial f_0}{\partial t} + L_0 f_0 + \frac{\partial \delta f}{\partial t} + \delta L f_0 + L_0 \delta f + \delta L \delta f = 0.$$

For fully kinetic ions, the propagators read

$$\begin{aligned}
L_{i0} &= \frac{1}{m_i} \left(p^\alpha - \frac{q_i}{c} A_0^\alpha \right) \frac{\partial}{\partial x^\alpha} \\
&- \frac{1}{2m_i} \left(p_\beta p_\gamma \frac{\partial g^{\beta\gamma}}{\partial x^\alpha} - \frac{2q_i}{c} p_\beta \frac{\partial A_0^\beta}{\partial x^\alpha} + \frac{q_i^2}{c^2} \frac{\partial A_0^2}{\partial x^\alpha} \right) \frac{\partial}{\partial p_\alpha}, \\
\delta L_i &= -\epsilon_\delta \frac{q_i}{cm_i} \delta A^\alpha \frac{\partial}{\partial x^\alpha} \\
&+ \epsilon_\delta q_i \left[\frac{1}{cm_i} \left(p_\beta \frac{\partial \delta A^\beta}{\partial x^\alpha} - \frac{q_i}{c} \frac{\partial A_{\beta 0} \delta A^\beta}{\partial x^\alpha} \right) - \frac{\partial \delta \phi}{\partial x^\alpha} \right] \frac{\partial}{\partial p_\alpha},
\end{aligned}$$

while for gyrokinetic electrons, the propagators are defined in gyrocenter phase space,

$$\begin{aligned}
L_{e0} &= \left(\frac{\bar{p}_{e\parallel}}{m_e} \frac{\mathbf{b}^*}{b_{\parallel}^*} + \epsilon_B \frac{c\bar{\mu}}{q_e B_{\parallel}^*} \hat{\mathbf{b}} \times \bar{\nabla} B_0 \right) \cdot \bar{\nabla} \\
&- \left(\bar{\mu} \frac{\mathbf{b}^*}{b_{\parallel}^*} \cdot \bar{\nabla} B_0 \right) \frac{\partial}{\partial \bar{p}_{e\parallel}}, \\
\delta L_e &= \epsilon_\delta \left(\frac{\partial \langle \delta \phi_{gc}^* \rangle}{\partial \bar{p}_{e\parallel}} \frac{\mathbf{b}^*}{b_{\parallel}^*} + \frac{c\hat{\mathbf{b}}}{B_{\parallel}^*} \times \bar{\nabla} \langle \delta \phi_{gc}^* \rangle \right) \cdot \bar{\nabla} \\
&- \frac{\epsilon_\delta \epsilon_{\parallel}}{\epsilon_B} q_e \frac{\mathbf{b}^*}{b_{\parallel}^*} \cdot \bar{\nabla} \langle \delta \phi_{gc}^* \rangle \frac{\partial}{\partial \bar{p}_{e\parallel}},
\end{aligned}$$

where the propagator δL_e contains terms of ordering ϵ_δ and $\epsilon_\delta \epsilon_{\parallel} / \epsilon_B$.

Instead of directly calculating the absolute changes in distribution δf_s , the perturbative δf simulation method [66] is utilized to minimize the particle statistical noise by calculating the evolution of particle weight function $W_s = \delta f_s / f_s$, where s denotes either ion species or electron species. Following the conventional δf method, the weight evolution equations dW_s/dt for ions and electrons can be easily derived as

$$\frac{dW_i}{dt} = \left(\frac{\partial}{\partial t} + L_i \right) \frac{\delta f_i}{f_i} = (W_i - 1) \delta L_i \ln f_{i0}, \quad (14)$$

$$\frac{dW_e}{dt} = \left(\frac{\partial}{\partial t} + L_e \right) \frac{\delta F_e}{F_e} = (W_e - 1) \delta L_e \ln F_{e0}, \quad (15)$$

where $L_s = L_{s0} + \delta L_s$ is the total propagator. If the equilibrium distribution has been chosen to be locally Maxwellian, equations (14) and (15) then become

$$\frac{dW_i}{dt} = (W_i - 1) \left[\dot{x}_1^\alpha \left(\kappa_i + \frac{\dot{p}_\alpha - \dot{p}_{\alpha 1}}{T_i} \right) - \dot{p}_{\alpha 1} \frac{\dot{x}^\alpha - \dot{x}_1^\alpha}{T_i} \right], \quad (16)$$

$$\frac{dW_e}{dt} = (W_e - 1) \left[\dot{\mathbf{X}}_1 \cdot \kappa_e - \dot{p}_{e\parallel 1} \frac{\bar{p}_{e\parallel}}{m_e T_e} \right], \quad (17)$$

where

$$\begin{aligned}
\kappa_i &= \frac{1}{n_{i0}} \frac{\partial n_{i0}}{\partial x^\alpha} + \frac{1}{T_i} \frac{\partial T_i}{\partial x^\alpha} \left(\frac{E_i}{T_i} - \frac{3}{2} \right), \\
\kappa_e &= \frac{\bar{\nabla} \bar{N}_{e0}}{\bar{N}_{e0}} - \frac{\bar{\mu}}{\bar{T}_e} \bar{\nabla} B_0 + \frac{\bar{\nabla} \bar{T}_e}{\bar{T}_e} \left(\frac{E_e}{\bar{T}_e} - \frac{3}{2} \right), \\
\dot{x}_1^\alpha &= -\epsilon_\delta \frac{q_i}{cm_i} \delta A^\alpha, \\
\dot{p}_1^\alpha &= \epsilon_\delta q_i \left[\frac{1}{cm_i} \left(p_\beta \frac{\partial \delta A^\beta}{\partial x^\alpha} - \frac{q_i}{c} \frac{\partial A_{\beta 0} \delta A^\beta}{\partial x^\alpha} \right) - \frac{\partial \delta \phi}{\partial x^\alpha} \right], \\
\dot{\mathbf{X}}_1 &= \epsilon_\delta \left(\frac{\partial \langle \delta \phi_{gc}^* \rangle}{\partial \bar{p}_{e\parallel}} \frac{\mathbf{b}^*}{b_{\parallel}^*} + \frac{c\hat{\mathbf{b}}}{B_{\parallel}^*} \times \bar{\nabla} \langle \delta \phi_{gc}^* \rangle \right), \\
\dot{p}_{e\parallel 1} &= -\frac{\epsilon_\delta \epsilon_{\parallel}}{\epsilon_B} q_e \frac{\mathbf{b}^*}{b_{\parallel}^*} \cdot \bar{\nabla} \langle \delta \phi_{gc}^* \rangle.
\end{aligned}$$

Now, a closed Vlasov–Maxwell system is constructed using the weight evolution equations, including equations (1) and (3) for full-f simulation or (16) and (17) for perturbative δf simulation, together with the gyrokinetic Poisson's equation (9) and Ampère's law (10).

8. Expressions in magnetic flux coordinate

In toroidal geometry, such as Tokamak or Stellarator geometry, it is convenient to introduce the toroidal magnetic flux coordinate system [67] (ψ_p, θ, ζ) , where ψ_p is the poloidal magnetic flux, θ is the poloidal angle, and ζ is the toroidal angle. In this coordinate system, it is very convenient to decompose a vector into components parallel and perpendicular to the direction of magnetic field to simplify the analysis, and the rapid particle motion along the lines is separated from the slow motion across the lines. The covariant and contravariant representation of unperturbed magnetic field

$$\begin{aligned}\mathbf{B}_0 &= \delta \nabla \psi_p + I \nabla \theta + g \nabla \zeta, \\ \mathbf{B}_0 &= q \nabla \psi_p \times \nabla \theta - \nabla \psi_p \times \nabla \zeta,\end{aligned}$$

and the covariant representation of unperturbed vector potential

$$\mathbf{A}_0 = \psi_t \nabla \theta - \psi_p \nabla \zeta,$$

accompanied by the Jacobian

$$\mathcal{J}^{-1} = \nabla \psi_p \cdot \nabla \theta \times \nabla \zeta = \frac{B_0^2}{I + gq},$$

construct the frame of the coordinate system, where ψ_t denotes the toroidal magnetic flux function, $q = d\psi_t/d\psi_p$ is the safety factor, and the radial component δ is very small and can be neglected.

In the magnetic flux coordinate system, the Hamilton's equations of ions are expressed as

$$\begin{aligned}\dot{\psi}_{pi} &= \frac{1}{m_i} \left(p^{\psi_p} - \frac{q_i}{c} \psi_p g^{\psi_p \theta} - \epsilon_\delta \frac{q_i}{c} \delta A^{\psi_p} \right), \\ \dot{\theta}_i &= \frac{1}{m_i} \left(p^\theta - \frac{q_i}{c} \psi_p g^{\theta \theta} - \epsilon_\delta \frac{q_i}{c} \delta A^\theta \right), \\ \dot{\zeta}_i &= \frac{1}{m_i} \left(p^\zeta + \frac{q_i}{c} \psi_p g^{\zeta \zeta} - \epsilon_\delta \frac{q_i}{c} \delta A^\zeta \right),\end{aligned}$$

$$\begin{aligned}\dot{p}_{\psi_p} &= \frac{-1}{2m_i} \left[p_{\psi_p} p_{\psi_p} \frac{\partial g^{\psi_p \psi_p}}{\partial \psi_p} + p_\theta p_\theta \frac{\partial g^{\theta \theta}}{\partial \psi_p} + 2p_{\psi_p} p_\theta \frac{\partial g^{\psi_p \theta}}{\partial \psi_p} \right. \\ &\quad - \frac{2q_i}{c} \left(q p_{\psi_p} g^{\psi_p \theta} + q p^\theta g^{\theta \theta} + \psi_p p_{\psi_p} \frac{\partial g^{\psi_p \theta}}{\partial \psi_p} - p_\zeta g^{\zeta \zeta} \right) \\ &\quad + \psi_p p_\theta \frac{\partial g^{\theta \theta}}{\partial \psi_p} \left. + \frac{q_i^2}{c^2} \left(\psi^2 \frac{\partial g^{\theta \theta}}{\partial \psi_p} + 2q \psi g^{\theta \theta} + 2\psi_p g^{\zeta \zeta} \right) \right. \\ &\quad - \epsilon_\delta \frac{2q_i}{c} \left(p_{\psi_p} \frac{\partial \delta A^{\psi_p}}{\partial \psi_p} + p_\theta \frac{\partial \delta A^\theta}{\partial \psi_p} + p_\zeta \frac{\partial \delta A^\zeta}{\partial \psi_p} \right) \\ &\quad \left. + \epsilon_\delta \frac{2q_i^2}{c^2} \left(q \delta A^\theta - \delta A^\zeta + \psi \frac{\partial \delta A^\theta}{\partial \psi_p} - \psi_p \frac{\partial \delta A^\zeta}{\partial \psi_p} \right) \right] - \epsilon_\delta q_i \frac{\partial \delta \phi}{\partial \psi_p},\end{aligned}$$

$$\begin{aligned}\dot{p}_\theta &= \frac{-1}{2m_i} \left[p_{\psi_p} p_{\psi_p} \frac{\partial g^{\psi_p \psi_p}}{\partial \theta} + 2p_{\psi_p} p_\theta \frac{\partial g^{\psi_p \theta}}{\partial \theta} + p_\theta p_\theta \frac{\partial g^{\theta \theta}}{\partial \theta} \right. \\ &\quad - \frac{2q_i}{c} \left(\psi p_{\psi_p} \frac{\partial g^{\psi_p \theta}}{\partial \theta} + \psi p_\theta \frac{\partial g^{\theta \theta}}{\partial \theta} \right) + \frac{q_i^2}{c^2} \psi^2 \frac{\partial g^{\theta \theta}}{\partial \theta} \\ &\quad - \epsilon_\delta \frac{2q_i}{c} \left(p_{\psi_p} \frac{\partial \delta A^{\psi_p}}{\partial \theta} + p_\theta \frac{\partial \delta A^\theta}{\partial \theta} + p_\zeta \frac{\partial \delta A^\zeta}{\partial \theta} \right) \\ &\quad \left. + \epsilon_\delta \frac{2q_i^2}{c^2} \left(\psi \frac{\partial \delta A^\theta}{\partial \theta} - \psi_p \frac{\partial \delta A^\zeta}{\partial \theta} \right) \right] - \epsilon_\delta q_i \frac{\partial \delta \phi}{\partial \theta},\end{aligned}$$

$$\begin{aligned}\dot{p}_\zeta &= \epsilon_\delta \frac{q_i}{cm_i} \left(p_{\psi_p} \frac{\partial \delta A^{\psi_p}}{\partial \zeta} + p_\theta \frac{\partial \delta A^\theta}{\partial \zeta} + p_\zeta \frac{\partial \delta A^\zeta}{\partial \zeta} \right) \\ &\quad - \epsilon_\delta \frac{q_i^2}{c^2 m_i} \left(\psi \frac{\partial \delta A^\theta}{\partial \zeta} - \psi_p \frac{\partial \delta A^\zeta}{\partial \zeta} \right) - \epsilon_\delta q_i \frac{\partial \delta \phi}{\partial \zeta},\end{aligned}$$

where the non-orthogonal components of the gauge tensor, such as $g^{\psi_p \zeta}$ and $g^{\theta \zeta}$ are null. It should be noted that the basis vector of perturbed vector potential $\delta \mathbf{A}$ is \mathbf{e}_α or \mathbf{e}^α , and the generalized velocity \dot{x}^β denotes angular velocity and linear velocity. In addition, the canonical momentum contains angular momentum terms, and the toroidal canonical momentum \mathbf{p}_ζ is conserved up to $\mathcal{O}(\epsilon)$. If we only consider the evolution of $\partial \ln f_{i0} / \partial \zeta^\alpha$ over ψ_p , then we can rewrite equation (16) as

$$\frac{dW_i}{dt} = (W_i - 1) \left[-\frac{q_i}{cm_i} \delta A^{\psi_p} \left(\kappa_{i\psi_p} + \frac{\dot{p}_{\psi_p} - \dot{p}_{\psi_p 1}}{m_i T_i} \right) - \frac{\dot{p}_{\alpha 1}}{T_i} (\dot{\zeta}^\alpha - \dot{\zeta}_i^\alpha) \right], \quad (18)$$

where the Einstein summation convention is applied over α , which can be any one of ψ_p, θ, ζ ,

$$\kappa_{i\psi_p} = \frac{1}{n_{i0}} \frac{\partial n_{i0}}{\partial \psi_p} + \frac{1}{T_i} \frac{\partial T_i}{\partial \psi_p} \left(\frac{E_i}{T_i} - \frac{3}{2} \right),$$

$$\dot{\zeta}_i^\alpha = -\epsilon_\delta \frac{q_i}{cm_i} \delta A^\alpha,$$

$$\begin{aligned}\dot{p}_{\psi_p 1} &= \epsilon_\delta \frac{q_i}{cm_i} \left[\left(p_{\psi_p} \frac{\partial \delta A^{\psi_p}}{\partial \psi_p} + p_\theta \frac{\partial \delta A^\theta}{\partial \psi_p} + p_\zeta \frac{\partial \delta A^\zeta}{\partial \psi_p} \right) \right. \\ &\quad \left. - \frac{q_i}{c} \left(q \delta A^\theta - \delta A^\zeta + \psi \frac{\partial \delta A^\theta}{\partial \psi_p} - \psi_p \frac{\partial \delta A^\zeta}{\partial \psi_p} \right) \right] - \epsilon_\delta q_i \frac{\partial \delta \phi}{\partial \psi_p},\end{aligned}$$

$$\begin{aligned}\dot{p}_{\theta 1} &= \epsilon_\delta \frac{q_i}{cm_i} \left[\left(p_{\psi_p} \frac{\partial \delta A^{\psi_p}}{\partial \theta} + p_\theta \frac{\partial \delta A^\theta}{\partial \theta} + p_\zeta \frac{\partial \delta A^\zeta}{\partial \theta} \right) \right. \\ &\quad \left. - \frac{q_i}{c} \left(\psi \frac{\partial \delta A^\theta}{\partial \theta} - \psi_p \frac{\partial \delta A^\zeta}{\partial \theta} \right) \right] - \epsilon_\delta q_i \frac{\partial \delta \phi}{\partial \theta},\end{aligned}$$

$$\dot{p}_{\zeta 1} = \dot{p}_\zeta.$$

Similarly, for electron species, the Hamilton's equations (4) and (5) in magnetic flux coordinate system are expressed as

$$\mathbf{B}_0^* = \left(1 - \epsilon_B \frac{B_0 \bar{p}_{e\parallel}}{m_e \Omega_{e0}} \frac{\partial}{\partial \psi_p} \frac{g}{B_0}\right) \nabla \zeta \times \nabla \psi_p \\ + \left(q + \epsilon_B \frac{B_0 \bar{p}_{e\parallel}}{m_e \Omega_{e0}} \frac{\partial}{\partial \psi_p} \frac{I}{B_0}\right) \nabla \psi_p \times \nabla \theta,$$

$$\dot{\psi}_{pe} = \epsilon_B \frac{c \bar{\mu}}{q_e D} \left(I \frac{\partial B_0}{\partial \zeta} - g \frac{\partial B_0}{\partial \theta}\right) + \epsilon_\delta \frac{c}{D} \left(I \frac{\partial \langle \delta \phi_{gc}^* \rangle}{\partial \zeta} - g \frac{\partial \langle \delta \phi_{gc}^* \rangle}{\partial \theta}\right),$$

$$\dot{\theta}_e = \frac{B_0}{D} \left(\frac{\bar{p}_{e\parallel}}{m_e} + \epsilon_\delta \frac{\partial \langle \delta \phi_{gc}^* \rangle}{\partial p_{e\parallel}}\right) \left(1 - \epsilon_B \frac{B_0 \bar{p}_{e\parallel}}{m_e \Omega_{e0}} \frac{\partial}{\partial \psi_p} \frac{g}{B_0}\right) \\ + \epsilon_B \frac{c g \bar{\mu}}{q_e D} \frac{\partial B_0}{\partial \psi_p} + \epsilon_\delta \frac{c g}{D} \frac{\partial \langle \delta \phi_{gc}^* \rangle}{\partial \psi_p},$$

$$\dot{\zeta}_e = \frac{B_0}{D} \left(\frac{\bar{p}_{e\parallel}}{m_e} + \epsilon_\delta \frac{\partial \langle \delta \phi_{gc}^* \rangle}{\partial p_{e\parallel}}\right) \left(q + \epsilon_B \frac{B_0 \bar{p}_{e\parallel}}{m_e \Omega_{e0}} \frac{\partial}{\partial \psi_p} \frac{I}{B_0}\right) \\ - \epsilon_B \frac{c I \bar{\mu}}{q_e D} \frac{\partial B_0}{\partial \psi_p} - \epsilon_\delta \frac{c I}{D} \frac{\partial \langle \delta \phi_{gc}^* \rangle}{\partial \psi_p},$$

$$\dot{\bar{p}}_{e\parallel} = \frac{B_0 \bar{\mu}}{D} \left[\left(\epsilon_B \frac{B_0 \bar{p}_{e\parallel}}{m_e \Omega_{e0}} \frac{\partial}{\partial \psi_p} \frac{g}{B_0} - 1 \right) \frac{\partial B_0}{\partial \theta} \right. \\ \left. - \left(q + \epsilon_B \frac{B_0 \bar{p}_{e\parallel}}{m_e \Omega_{e0}} \frac{\partial}{\partial \psi_p} \frac{I}{B_0} \right) \frac{\partial B_0}{\partial \zeta} \right] - \epsilon_\delta \frac{q_e B_0}{D} \\ \left[\left(1 - \epsilon_B \frac{B_0 \bar{p}_{e\parallel}}{m_e \Omega_{e0}} \frac{\partial}{\partial \psi_p} \frac{g}{B_0} \right) \frac{\partial \langle \delta \phi_{gc}^* \rangle}{\partial \theta} \right. \\ \left. + \left(q + \epsilon_B \frac{B_0 \bar{p}_{e\parallel}}{m_e \Omega_{e0}} \frac{\partial}{\partial \psi_p} \frac{I}{B_0} \right) \frac{\partial \langle \delta \phi_{gc}^* \rangle}{\partial \zeta} \right],$$

$$D = I + gq + \epsilon_B \frac{B_0 \bar{p}_{e\parallel}}{m_e \Omega_{e0}} \left(g \frac{\partial}{\partial \psi_p} \frac{I}{B_0} - I \frac{\partial}{\partial \psi_p} \frac{g}{B_0} \right).$$

The electron weight evolution equation (17) can be rewritten as

$$\frac{dW_e}{dt} = (W_e - 1) \left(\dot{\psi}_{pe1} \kappa_e \psi_p - \dot{\bar{p}}_{e\parallel 1} \frac{\bar{p}_{e\parallel}}{m_e \bar{T}_e} \right), \quad (19)$$

where

$$\kappa_e \psi_p = \frac{1}{\bar{N}_{e0}} \frac{\partial \bar{N}_{e0}}{\partial \psi_p} + \frac{1}{\bar{T}_e} \frac{\partial \bar{T}_e}{\partial \psi_p} \left(\frac{E_e}{\bar{T}_e} - \frac{3}{2} \right) - \frac{\bar{\mu}}{\bar{T}_e} \frac{\partial B_0}{\partial \psi_p},$$

$$\dot{\psi}_{pe1} = \epsilon_\delta \frac{c}{D} \left(I \frac{\partial \langle \delta \phi_{gc}^* \rangle}{\partial \zeta} - g \frac{\partial \langle \delta \phi_{gc}^* \rangle}{\partial \theta} \right),$$

$$\dot{\bar{p}}_{e\parallel 1} = -\epsilon_\delta \frac{q_e B_0}{D} \left[\left(1 - \epsilon_B \frac{B_0 \bar{p}_{e\parallel}}{m_e \Omega_{e0}} \frac{\partial}{\partial \psi_p} \frac{g}{B_0} \right) \frac{\partial \langle \delta \phi_{gc}^* \rangle}{\partial \theta} \right. \\ \left. + \left(q + \epsilon_B \frac{B_0 \bar{p}_{e\parallel}}{m_e \Omega_{e0}} \frac{\partial}{\partial \psi_p} \frac{I}{B_0} \right) \frac{\partial \langle \delta \phi_{gc}^* \rangle}{\partial \zeta} \right].$$

Note that the basis vector of covariant gyrocenter velocity is not $\nabla \xi^\beta \times \nabla \xi^\gamma$ but \mathbf{e}_α .

In curvilinear coordinate system, the rigorous expression for Laplacian operator ∇^2 is very complicated, especially for perpendicular operator ∇_\perp^2 . But in the field-aligned coordinate system $(\psi_p, \theta_0, \zeta_0)$ [68], where $\theta_0 = \theta - \zeta/q$, $\zeta_0 = \zeta$, the operator ∇_\perp^2 can be reduced to two dimensions. The perpendicular Laplacian operator in the new coordinates has the same Jacobian to magnetic flux coordinate,

$$\nabla_\perp^2 = g^{\psi_p \psi_p} \frac{\partial^2}{\partial \psi_p^2} + 2g^{\psi_p \theta_0} \frac{\partial^2}{\partial \psi_p \partial \theta_0} + \left(g^{\theta_0 \theta_0} + \frac{g^{\zeta \zeta}}{q^2} \right) \frac{\partial^2}{\partial \theta_0^2} \\ + \frac{1}{\mathcal{J}} \left(\frac{\partial \mathcal{J} g^{\psi_p \psi_p}}{\partial \psi_p} + \frac{\partial \mathcal{J} g^{\psi_p \theta_0}}{\partial \theta_0} \right) \frac{\partial}{\partial \psi_p} \\ + \frac{1}{\mathcal{J}} \left(\frac{\partial \mathcal{J} g^{\psi_p \theta_0}}{\partial \psi_p} + \frac{\partial \mathcal{J} g^{\theta_0 \theta_0}}{\partial \theta_0} \right) \frac{\partial}{\partial \theta_0}.$$

In this way, the gyrokinetic Poisson's equation in magnetic flux coordinate system becomes

$$\left(1 + \sum_e \frac{\omega_{pe}^2}{\Omega_e^2} \right) \nabla_\perp^2 \delta \phi + \sum_e \frac{4\pi q_e \bar{N}_{e0}}{B_0} \varepsilon^{\alpha\beta\gamma} \partial_\gamma \frac{\delta A_\alpha B_\beta}{B_0} \\ = -4\pi \left(\sum_i q_i \delta n_i + \sum_e q_e \delta \bar{N}_e \right), \quad (20)$$

where $\varepsilon^{\alpha\beta\gamma}$ is the Levi-Civita symbol, and its value is 0 or $\pm 1/\mathcal{J}$. And the expression of Ampere's law is given as follows

$$\left[- \left(1 + \sum_e \beta_{e0} \right) \nabla_\perp^2 \delta A^\gamma + \sum_i \frac{\omega_{pi}^2}{c^2} \delta A^\gamma \right. \\ \left. + \sum_e \left(\frac{\omega_{pe}^2}{c^2} + \beta_{e0} \nabla_\perp^2 \right) \frac{B_\tau \delta A^\tau B^\gamma}{B_0^2} \right] \mathbf{e}_\gamma \\ - \sum_e \varepsilon^{\alpha\beta\gamma} \left[\frac{4\pi q_e \bar{N}_{e0} B_\alpha}{B_0^2} \partial_\beta \delta \phi + \frac{6\pi c \bar{P}_{e0} B_\alpha}{B_0^3 \Omega_e} \partial_\beta \nabla_\perp^2 \delta \phi \right] \mathbf{e}_\gamma \\ = \frac{4\pi}{c} \delta J^\gamma \mathbf{e}_\gamma, \quad (21)$$

where

$$\delta J^\gamma = \sum_i \int (p_i^\gamma - A^\gamma) \delta f_i d^3 p_i + \sum_e \frac{B^\gamma}{B_0} \int q_e \frac{p_{e\parallel 0}}{m_e} \delta \bar{F}_e d^3 p_e \\ + \sum_e \varepsilon^{\alpha\beta\gamma} \frac{B_\alpha}{B_0} \partial_\beta \int c \mu_{e0} \delta \bar{F}_e d^3 p_e.$$

The contravariant components of unperturbed magnetic field are $B^{\psi_p} = 0$, $B^\theta = 1/\mathcal{J}$, and $B^\zeta = q/\mathcal{J}$, the covariant components of unperturbed magnetic field are $B_{\psi_p} = \delta$, $B_\theta = I$, and $B_\zeta = g$.

The weight evolution equations (18) and (19) (for perturbative δf simulation) together with the gyrokinetic Poisson's equation (20) and the Ampère's law (21) construct a closed Vlasov–Maxwell system with a local Maxwellian distribution in the magnetic flux coordinate system.

9. Discussion

In this work, the Lie-transform perturbation theory for Hamiltonian system [47–51] is applied to construct a closed Vlasov–Maxwellian simulation model suitable for code development in toroidal geometry. The scalar potential and vector potential are directly solved using the gyrokinetic Poisson’s equation and Ampère’s law, which avoids intermediate variables and equations for better performance and numerical properties. The application of Hamiltonian mechanics insures that the total energy of the Vlasov–Maxwell system is conserved, which is the basic prerequisite for the construction of a simulation model.

By comparison with GeFi, the closure approach of simulation model is obviously different. Moreover, the direct solution of Poisson’s equation and Ampère’s law is more compact. If the parallel magnetic field is used instead of the perpendicular vector potential, another alternative form of Poisson’s equation and Ampère’s law is obtained in terms of δA_{\parallel} and δB_{\parallel} . In slab geometry, the perpendicular Ampère’s law naturally holds the ‘so-called pressure balance equation’ [59], which takes the exact form of the force balance equation used in GeFi [39], except as otherwise noted in section 5: the reduced perpendicular Ampère’s Law is quantitatively different from the counterpart of GeFi in that the coefficient of $c\bar{P}_{e0}\nabla_{\perp}^2\delta\phi/(B_0\Omega_e)$ is 3/2 in the current model whereas it is 1 in the GeFi model.

Since the ordering parameters ϵ_B , ϵ_{ω} , ϵ_{δ} and ϵ_{\parallel} are retained for the sake of the convenience of ordering analysis and truncation, various ordering relationships among these four parameters can easily be chosen for physical processes with different spatial and temporal scales. Therefore, the final gyrokinetic Vlasov equations and field equations can readily be obtained by choosing the actual ordering parameters.

10. Conclusion

An energy conservation Vlasov–Maxwell model, which includes a fully kinetic description for heavy ion species and a gyrokinetic description for light electron species, has been developed using the mature Lie-transform perturbation theory for Hamiltonian systems. The generic form is then cast into magnetic flux coordinate system with local Maxwellian equilibrium distributions for both ion species and electron species. This closed model consists of the distribution equations in either full- f or δf form, gyrokinetic Poisson’s equation and Ampère’s law.

As the ion cyclotron motion is retained and electrons are described using gyrokinetic theory, this model is capable of investigating collisionless dynamic processes ranging from ion cyclotron frequency to lower hybrid frequency, such as the propagation property of ICRF waves and LHW, and the energy absorption of RF waves.

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Appendix. Tensor analysis in curvilinear coordinate system

In previous sections, the expression of motion equations in magnetic flux coordinate utilizes tensor analysis in a curvilinear coordinate system. If, in a Cartesian coordinate system (x^1, x^2, x^3) , the basis vectors are prescribed as \mathbf{j}_1 , \mathbf{j}_2 , and \mathbf{j}_3 , then an arbitrary vector \mathbf{R} can be written as

$$\mathbf{R} = x^1\mathbf{j}_1 + x^2\mathbf{j}_2 + x^3\mathbf{j}_3.$$

In a curvilinear coordinate system, vectors can either be defined as a set of contravariant basis vectors \mathbf{u}^1 , \mathbf{u}^2 , and \mathbf{u}^3 associated with the corresponding covariant components (ξ_1, ξ_2, ξ_3) , or a set of covariant basis vectors \mathbf{u}_1 , \mathbf{u}_2 , and \mathbf{u}_3 linked with their contravariant components (ξ^1, ξ^2, ξ^3) , then the position vector \mathbf{R} may have two kinds of representations,

$$\mathbf{R} = \xi_1\mathbf{u}^1 + \xi_2\mathbf{u}^2 + \xi_3\mathbf{u}^3,$$

$$\mathbf{R} = \xi^1\mathbf{u}_1 + \xi^2\mathbf{u}_2 + \xi^3\mathbf{u}_3.$$

The covariant basis vector \mathbf{u}_1 is parallel to $\mathbf{u}^2 \times \mathbf{u}^3$, \mathbf{u}_2 parallel to $\mathbf{u}^3 \times \mathbf{u}^1$, and \mathbf{u}_3 parallel to $\mathbf{u}^1 \times \mathbf{u}^2$.

In a Cartesian coordinate system, the unit basis vectors are independent of space and time, so the time derivative of \mathbf{R} can be written as

$$\frac{d\mathbf{R}}{dt} = \frac{dx^1}{dt}\mathbf{j}_1 + \frac{dx^2}{dt}\mathbf{j}_2 + \frac{dx^3}{dt}\mathbf{j}_3.$$

But in curvilinear coordinates, the basis vectors are wavering vectors in general, therefore

$$d\mathbf{R} \neq d\xi^1\mathbf{u}_1 + d\xi^2\mathbf{u}_2 + d\xi^3\mathbf{u}_3.$$

The time derivative of the basis vectors should thus be considered,

$$\frac{d\mathbf{R}}{dt} = \frac{d\xi^i}{dt}\mathbf{u}_i + \xi^i\frac{d\mathbf{u}_i}{dt}.$$

Since we treat \mathbf{R} as a position vector, then the time derivative $d\mathbf{R}/dt$ is the velocity vector. If one wants to calculate the time derivative of velocity vector or kinetic energy, the procedure may be very tedious. From another point of view, this difficulty can be overcome according to the following justifiable equations,

$$d\mathbf{R} = \frac{\partial\mathbf{R}}{\partial\xi^1}d\xi^1 + \frac{\partial\mathbf{R}}{\partial\xi^2}d\xi^2 + \frac{\partial\mathbf{R}}{\partial\xi^3}d\xi^3,$$

$$d\mathbf{R} = \frac{\partial\mathbf{R}}{\partial\xi_1}d\xi_1 + \frac{\partial\mathbf{R}}{\partial\xi_2}d\xi_2 + \frac{\partial\mathbf{R}}{\partial\xi_3}d\xi_3.$$

Two sets of new basic vectors will then be defined in terms of the covariant basis vectors

$$\frac{\partial \mathbf{R}}{\partial \xi^\alpha} = \mathbf{e}_\alpha$$

and the contravariant basis vectors

$$\frac{\partial \mathbf{R}}{\partial \xi^\beta} = \mathbf{e}^\beta = \nabla \xi^\beta.$$

In this way, two new types of representations of vector velocity are given:

$$\mathbf{V} = \frac{d\mathbf{R}}{dt} = \dot{\xi}^\alpha \mathbf{e}_\alpha = V^\alpha \mathbf{e}_\alpha,$$

$$\mathbf{V} = \frac{d\mathbf{R}}{dt} = \dot{\xi}_\alpha \mathbf{e}^\alpha = V_\alpha \mathbf{e}^\alpha.$$

It should be noted that the basis vectors \mathbf{e}_α and \mathbf{e}^α are different from \mathbf{u}_α and \mathbf{u}^α . In curvilinear coordinate system, the contravariant and covariant gauge tensor and Jacobian are defined as

$$g^{\alpha\beta} = \mathbf{e}^\alpha \cdot \mathbf{e}^\beta, g_{\alpha\beta} = \mathbf{e}_\alpha \cdot \mathbf{e}_\beta,$$

$$\mathcal{J} = \mathbf{e}_1 \cdot (\mathbf{e}_2 \times \mathbf{e}_3)$$

with

$$\mathbf{e}_\alpha \cdot \mathbf{e}^\beta = \delta_\alpha^\beta, \mathbf{e}_\alpha = g_{\alpha\nu} \mathbf{e}^\nu,$$

$$\nabla \xi^\beta \times \nabla \xi^\gamma = \varepsilon^{\alpha\beta\gamma} \mathbf{e}_\alpha.$$

The expression of the space differential operator ∇ in a curvilinear coordinate system can be converted from that in Cartesian coordinate system

$$\nabla = \frac{\partial}{\partial x^i} \mathbf{j}^i = \frac{\partial}{\partial \xi^\alpha} \frac{\partial \xi^\alpha}{\partial x^i} \mathbf{j}^i = \frac{\partial}{\partial \xi^\alpha} \nabla \xi^\alpha,$$

$$\nabla^2 = \frac{1}{\sqrt{g}} \partial_\alpha \left(\sqrt{g} g^{i\alpha} \partial_i \right),$$

where $\partial_\alpha = \partial/\partial \xi^\alpha$. The exact form of the spacial differential operator ∇_\perp and the perpendicular Laplacian operator ∇_\perp^2 are

$$\nabla_\perp = \nabla - \hat{\mathbf{b}} \left(\hat{\mathbf{b}} \cdot \nabla \right) = \mathbf{e}^\alpha \partial_\alpha - \mathbf{e}_\beta \frac{B^\beta B^\gamma}{B_0^2} \partial_\gamma = \mathbf{e}^i \partial_i - \mathbf{e}^j \frac{B_j B^k}{B_0^2} \partial_k,$$

$$\nabla_\perp^2 = \left(\mathbf{e}^\alpha \partial_\alpha - \mathbf{e}^\beta \frac{B_\beta B^\gamma}{B_0^2} \partial_\gamma \right) \cdot \left(\mathbf{e}^i \partial_i - \mathbf{e}^j \frac{B_j B^k}{B_0^2} \partial_k \right).$$

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