Bounce-Averaged Kinetic Equations and Neoclassical Polarization Density

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Abstract

The rigorous formulation of the bounce-averaged equations is presented based upon the Poincaré-Cartan one-form and Lie perturbation methods. The resulting bounce-averaged Vlasov equation is Hamiltonian, thus suitable for the self-consistent simulation of low frequency electrostatic turbulence in the trapped ion mode regime. In the bounce-kinetic Poisson equation, the "neoclassical polarization density" arises from the difference between bounce-averaged banana center and real trapped particle densities across a field line. This representation of the neoclassical polarization drift as a shielding term provides a systematic way to study the long term behavior of the turbulence driven $\mathbf{E} \times \mathbf{B}$ flow.

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I. INTRODUCTION

The reduced kinetic description of plasma dynamics based on the existence of adiabatic invariants has contributed greatly to the theoretical development of magnetic confinement physics. The best example is the nonlinear gyrokinetic formalism[1–6] which describes fluctuations with characteristic frequency ω much lower than the ion cyclotron frequency Ω_{ci} such that the first adiabatic invariant μ is conserved. It has provided a rigorous foundation for analytical kinetic microturbulence models,[7,8] gyrokinetic particle-in-cell simulations,[9–14] and the development of nonlinear gyrofluid equations[15–19] for tokamak plasmas. Even with overly simplified electron dynamics, nonlinear gyrokinetic and gyrofluid simulations of ion temperature gradient driven turbulence have reproduced many features of turbulence often found in tokamak plasmas.

The nonlinear bounce-averaged kinetic equation for trapped electrons,[20] which relies on the conservation of the second adiabatic invariant J in addition to μ, for fluctuations with characteristic frequency lower than the bounce frequency of the mirror trapped electrons (ω_{Be}), offers a more realistic description of the electron dynamics. Nonlinear kinetic theories of trapped electron driven turbulence[7,5] based on this formalism have demonstrated the possibility of reproducing some of the confinement trends of Ohmic and Supershot plasmas. It is also worthwhile to note that the bounce-averaged kinetic equation has been useful in studying low frequency instabilities in the earth's dipole field.[21]

Previous bounce-averaged kinetic equations have been derived in the limit of vanishing radial width of the banana orbit. In this work, we include the full banana orbit width in the bounce-averaged kinetic formalism to provide a firm theoretical foundation for the description of low frequency large scale fluctuations such as the trapped ion mode,[22,23] turbulence driven $\mathbf{E} \times \mathbf{B}$ flow[24,25] (the axisymmetric mode), and convective cells.[26] Indeed, from reflectometry[27] and beam emission spectroscopy measurements[28] on the Tokamak Fusion Test Reactor (TFTR),[29] one observes that a significant fraction of the fluctuation intensity resides in the trapped ion mode regime corresponding to $\omega < \omega_{Bi}$, the bounce frequency of mirror trapped ions. From the theoretical side, both a comprehensive kinetic code calculation[30] and nonlinear simulations[11,15,14,31] show the importance of long wavelength low frequency fluctuations. Persistent appearance of Bohm-like scaling of large tokamak transport[32–34] has also revived theoretical studies[35–37] of trapped ion driven turbulence. Finally, small radial scale fluctuating $\mathbf{E} \times \mathbf{B}$ flow driven by turbulence (zonal flow) has been observed in both nonlinear gyrofluid[38–41] and gyrokinetic[13,31] simulations, as well as at the DIII-D tokamak edge.[42] It has been shown that the long term asymptotic behavior of this zonal flow can be addressed by the bounce-kinetic equation.[43]

In analogy to gyrokinetics, the formalism of one-form mechanics and Lie perturbation theory is employed.[44–46] The formalism has convenient transformation properties and allows us to preserve the Hamiltonian structure explicitly. We adopt three small quantities for our ordering scheme: ϵ_B, which measures the ratio of the ion banana radius Λ_B to the equilibrium magnetic field gradient scale length, $L_B \sim B/|\nabla B|$; in analogy to the gyrokinetic ordering, $\epsilon_\phi \sim e\phi/T_i \sim 1/k_\perp L_p$, where L_p is the pressure gradient scale length; and $\epsilon_k \sim \omega/\omega_B \sim k_\perp \Lambda_B$, where ω_B is the ion bounce frequency. The first two parameters are analogous to the corresponding small parameters in gyrokinetics, whereas the ϵ_k ordering, corresponding to the low frequency limit, is necessary to ensure the adiabatic invariance of the bounce action. In addition, long parallel wavelength perturbations are assumed, i.e., $k_\parallel \ll k_\perp$. Because the bounce phase angle dependence arises only in perturbed quantities, one can apply Lie perturbation theory[44,47,48,45] to remove systematically this phase dependence to any desired order, while also preserving the Hamiltonian structure of the equations.

The principal results of this paper are as follows:

i) The nonlinear electrostatic bounce-averaged kinetic equations are derived systematically. A symplectic derivation via phase-space Lagrangian Lie-perturbation theory ensures the preservation of the Hamiltonian structure and conservation laws.

ii) The full banana orbit width effect is retained in both bounce-averaged Vlasov and Poisson equations. In the bounce-kinetic Poisson equation, the general form of the neoclassical polarization density is obtained. This can provide useful insights into the long term behavior

of the turbulence driven $\mathbf{E} \times \mathbf{B}$ flow.
iii) The relationship between the neoclassical polarization density associated with the difference between the real trapped particle density and the bounce-averaged banana center density, and the more familiar neoclassical polarization drift[49,50,43] is elucidated.
The formalism presented in this paper should be useful for bounce-kinetic particle-in-cell simulations of trapped particle modes.

The remainder of this paper is organized as follows: in Section II we review the reduced motion described by the guiding center drift equations and provide an heuristic estimate of the neoclassical polarization density. The formalism of one-form mechanics and coordinate transformations is summarized in Section III. In Section IV we derive the Vlasov equation in bounce-averaged coordinates for a simple circular cross-section tokamak equilibrium. In Section V, we derive the bounce-kinetic Poisson equation and the general form of the neoclassical polarization density. Finally, in Section VI we provide a summary and discussion of our work.

II. REVIEW OF GUIDING CENTER MOTION AND AN HEURISTIC ESTIMATE OF NEOCLASSICAL POLARIZATION DENSITY

In order to provide a simple physical picture of the bounce motion and neoclassical polarization density, we review and extend the guiding center treatment of trapped particle motion in high aspect ratio ($\epsilon_a \ll 1$) tokamaks given by Kadomtsev and Pogutse.[51] A simple heuristic estimate will be given for the neoclassical polarization density based upon both the radial and toroidal deviations of the guiding center from the center of the bounce motion. The equilibrium guiding center drift equation is

$$\mathbf{v} = v_\parallel \mathbf{b} + \frac{mc(v_\perp^2 + 2v_\parallel^2)}{2eB^3}\mathbf{B} \times \nabla B, \tag{1}$$

which, together with the conservation of the magnetic moment, μ, and energy, E, completely determines the guiding center motion. For the equilibrium field, we take

$$\mathbf{B} = \frac{\epsilon_a B_0}{q(1+\epsilon_a \cos\theta)}\hat{\theta} + \frac{B_0}{1+\epsilon_a\cos\theta}\hat{\zeta}; \tag{2}$$

here $\epsilon_a = r/R_0$ is the local inverse aspect ratio and q is the magnetic safety factor. In toroidal coordinates (r,θ,ζ), we have to lowest order

$$\frac{dr}{dt} \approx -\frac{(v^2+v_\parallel^2)}{2\Omega_c R_0}\sin\theta, \tag{3}$$

$$\frac{d\theta}{dt} \approx \frac{v_\parallel}{R_0 q} - \frac{(v^2+v_\parallel^2)}{2\Omega_c r R_0}\cos\theta, \tag{4}$$

$$\frac{d\zeta}{dt} \approx \frac{v_\parallel}{R_0}, \tag{5}$$

where we have neglected terms higher order in ϵ_a. Upon integrating these equations as functions of θ, we obtain

$$r(\theta) = r_0 \pm \frac{v q_0}{\Omega_c\sqrt{\epsilon_a}}\left(\frac{v_{\parallel 0}^2}{\epsilon_a v_{\perp 0}^2} - 2\sin^2\frac{\theta}{2}\right)^{\frac{1}{2}}, \tag{6}$$

where r_0 is the radius of the bounce points, q_0 is the safety factor evaluated at r_0, and $v_{\parallel 0}$ and $v_{\perp 0}$ are the velocity components at the outer mid-plane of the torus. Here we introduce the banana radius $\Lambda_B \equiv vq_0/\Omega_c\sqrt{\epsilon_a}$ and the pitch angle $\kappa^2 \equiv v_{\parallel 0}^2/2\epsilon_a v_{\perp 0}^2$. Trapping corresponds to $\kappa^2 \le 1$, and for small ϵ_a this implies $v_{\parallel 0}^2 \ll v_{\perp 0}^2$ (thus $v_{\perp 0} \approx v$). In the poloidal plane, the guiding center motion can be viewed in terms of a bounce center at r_0 with the second term representing the periodic bounce motion. The upper sign applies when the motion is in the positive sense of $\hat{\zeta}$ (the first half of the orbit) and the lower sign for the opposite direction (the second half of the orbit).

The motion in the toroidal direction is given by

$$\zeta(\theta) = q_0\theta + \sqrt{2}\,\Lambda_B\left[\left(2q_0' + \frac{q_0}{r_0}\right)C_1(\varphi(\theta),\kappa) - \left(2q_0'(1-\kappa^2) + \frac{q_0}{2r_0}\right)C_2(\varphi(\theta),\kappa)\right] \tag{7}$$

where

$$C_1(\varphi(\theta),\kappa) = \begin{cases} E(\varphi,\kappa) + \mathbf{E}(\kappa) & \text{first half of orbit} \\ 3\mathbf{E}(\kappa) - E(\varphi,\kappa) & \text{second half of orbit} \end{cases} \tag{8}$$

$$C_2(\varphi(\theta),\kappa) = \begin{cases} F(\varphi,\kappa) + \mathbf{K}(\kappa) & \text{first half of orbit} \\ 3\mathbf{K}(\kappa) - F(\varphi,\kappa) & \text{second half of orbit,} \end{cases} \tag{9}$$

and

$$\varphi(\theta) \equiv \arcsin\left(\frac{\sin(\theta/2)}{\kappa}\right). \tag{10}$$

$F(\varphi, \kappa)$ and $E(\varphi, \kappa)$ are elliptic integrals of the first and second kind, respectively; $\mathbf{K}(\kappa)$ and $\mathbf{E}(\kappa)$ are the corresponding complete elliptic integrals; primes refer to $\partial/\partial r$. φ is similar to a phase angle of the trapped particle bounce motion but is only defined between $-\pi/2$ to $\pi/2$. The separation of the bounce motion and the averaged motion in the toroidal direction is not as simple as it is for the radial motion. Unlike $r(\theta)$, the toroidal position does not return to its original value after a complete orbit. The difference in the poloidal angular velocity between the first and second halves of the orbit, due to the effects of the magnetic field strength inhomogeneity and curvature along with the magnetic shear, gives rise to a net precessional motion in the toroidal direction. Since the guiding center motion follows the field line to lowest order, the separation of average and bounce motions can be seen more easily in flux coordinates rather than toroidal coordinates.[52] The bounce motion is thus mostly along the field line with deviations in the $\beta \equiv \psi_p(r)$ (radial) direction and $\alpha \equiv \zeta - q(r)\theta$ ($\sim$ non-radial perpendicular) direction. Then, we can define an average precessional motion by means of the average precession frequency,

$$\omega_{pr} = \frac{\alpha(\theta_f) - \alpha(\theta_i)}{\tau_B}, \tag{11}$$

where τ_B is the bounce period. The α position of the bounce center is given by $\alpha_{pr}(\theta) \equiv \omega_{pr} t(\theta)$, where we have integrated $dt/d\theta$ to find t as a function of θ; the deviation from the average is $\Delta\alpha(\theta) \equiv \alpha(\theta) - \omega_{pr} t(\theta)$,

$$\Delta\alpha(\theta) = \mp\sqrt{2}\,\Lambda_B \left[\left(2q_0' + \frac{q_0}{r_0}\right)\left(\frac{\mathbf{E}(\kappa)}{\mathbf{K}(\kappa)} F(\varphi, \kappa) - E(\varphi, \kappa)\right) + q_0'\theta\left(\kappa^2 - \sin^2(\theta/2)\right)^{1/2}\right]. \tag{12}$$

Thus, the motion of the guiding center is given by

$$r(\theta) = r_0 + \Delta r(\theta) \tag{13}$$

$$\alpha(\theta) = \alpha_{pr}(\theta) + \Delta\alpha(\theta), \tag{14}$$

while the motion of the bounce center is simply $(r_0, \alpha_{pr}(\theta))$. One can now readily see the separation between the averaged and bounce motions.

Before we present an heuristic derivation of the neoclassical polarization density, we first review the role and origin of the classical polarization density in gyrokinetics.[2] The classical polarization density arises directly from the effect of the polarization drift of the ions. In addition, the density is associated with the difference between the real particle density and the gyroaveraged particle density. That is, if

$$\mathbf{v}_{pol} = \frac{c}{\Omega_c B}\frac{\partial \mathbf{E}_\perp}{\partial t} = \frac{mc^2}{eB^2}\frac{\partial \mathbf{E}_\perp}{\partial t}, \tag{15}$$

then the induced polarization current density is simply

$$\begin{aligned} \mathbf{j}_{pol} &= en_{i0}\mathbf{v}_{i,pol} - en_{e0}\mathbf{v}_{e,pol} \\ &\approx \frac{n_{i0}m_i c^2}{eB^2}\frac{\partial \mathbf{E}_\perp}{\partial t}, \end{aligned} \tag{16}$$

and using the continuity equation, the polarization density is

$$n_{pol} = \frac{4\pi m_i c^2}{eB^2}\nabla_\perp \cdot (n_{i0}\nabla_\perp \phi). \tag{17}$$

Representing the polarization drift as a shielding term in the gyrokinetic Poisson equation has provided one of the principal computational advantages of the gyrokinetic approach.[2] We expect that the neoclassical polarization density will arise from the modification of the classical polarization drift due to the toroidal magnetic geometry.

To give an heuristic estimate of the neoclassical polarization density as the difference between the real trapped particle density and the bounce-averaged banana center density, we define the bounce-average of a quantity g to be

$$\langle g(\theta)\rangle_\theta = \frac{\oint g(\theta)\frac{dt}{d\theta}d\theta}{\oint \frac{dt}{d\theta}d\theta} = \frac{\oint \frac{qR}{v_\parallel}g(\theta)d\theta}{\tau_B}. \tag{18}$$

To calculate the bounce-averaged density we need the first two θ-moments of $\Delta r(\theta)$ and $\Delta\alpha(\theta)$. As expected, $\langle \Delta r(\theta)\rangle_\theta$ and $\langle \Delta\alpha(\theta)\rangle_\theta$ are zero; the average motion has already explicitly been separated from the bounce motion. For $\langle(\Delta r(\theta))^2\rangle_\theta$, $\langle(\Delta\alpha(\theta))^2\rangle_\theta$, and $\langle\Delta r\Delta\alpha\rangle_\theta$, we take the deeply-trapped particle limit and find

$$\langle(\Delta r(\theta))^2\rangle_\theta = \Lambda_B^2\kappa^2 \tag{19}$$

$$\langle(\Delta\alpha(\theta))^2\rangle_\theta = \frac{1}{16}\Lambda_B^2\left(2q_0' - \frac{q_o}{r_0}\right)^2\kappa^4 \tag{20}$$

$$\langle\Delta r\Delta\alpha\rangle_\theta = 0. \tag{21}$$

(Notice that the average toroidal deviation is smaller than the average radial deviation by a factor of the pitch angle; however, we will see that the lowest order contribution is really $\mathcal{O}(\kappa^2)$ in the rigorous bounce-averaged formulation.) Now we can calculate the difference between bounce-averaged and real particle densities. Expanding n_i about the bounce-center in flux coordinates, we have

$$\begin{aligned} n_i(\mathbf{X}+\mathbf{\Lambda}) \approx n_i(\mathbf{X}) \; + \; \Delta r(\theta)\frac{\partial n_i}{\partial r}\bigg|_{\mathbf{X}} + \Delta\alpha(\theta)\frac{\partial n_i}{\partial \alpha}\bigg|_{\mathbf{X}} + \\ \frac{(\Delta r)^2}{2}\frac{\partial^2 n_i}{\partial r^2}\bigg|_{\mathbf{X}} + \frac{(\Delta\alpha)^2}{2}\frac{\partial^2 n_i}{\partial \alpha^2}\bigg|_{\mathbf{X}} + \Delta r\Delta\alpha\frac{\partial^2 n_i}{\partial r\partial\alpha}\bigg|_{\mathbf{X}}. \end{aligned} \tag{22}$$

Bounce-averaging the expansion and integrating over the trapped particle portion of velocity space, we find

$$n_i(\mathbf{X}) - \langle\langle n_i(\mathbf{X}+\mathbf{\Lambda})\rangle_\theta\rangle_v \tag{23}$$

$$\begin{aligned} &\approx \frac{1}{4}\Lambda_{B,th}^2\sqrt{2\epsilon_a}\frac{n_{i0}e}{T_i}\frac{\partial^2\phi}{\partial r^2} \; + \; \frac{3}{320}\Lambda_{B,th}^2\left(2q_0' - \frac{q_0}{r_0}\right)^2\sqrt{2\epsilon_a}\frac{n_{i0}e\phi}{T_i}\frac{\partial^2\phi}{\partial\alpha^2} \\ &= \frac{1}{4}\frac{m_i n_{i0}c^2}{eB_p^2}(2\epsilon_a)^{3/2}\frac{\partial^2\phi}{\partial r^2} \; + \; \frac{3}{320}\frac{m_i n_{i0}c^2}{eB_p^2}\left(2q_0' - \frac{q_0}{r_0}\right)^2(2\epsilon_a)^{3/2}\frac{\partial^2\phi}{\partial\alpha^2}, \end{aligned} \tag{24}$$

where we have estimated that $\delta n_{i,\mathrm{trapped}} \sim \sqrt{2\epsilon_a}n_{i0}e\phi/T_i$ for $\omega \ll \omega_{Bi}$. The first term represents the contribution to the neoclassical polarization density due to the radial banana excursions while the second term is due to the α excursions. The radial part of the neoclassical polarization current has been derived before by Callen,[49] Callen obtains

$$\mathbf{j}_{pol} \approx \frac{16}{3\pi\sqrt{2}}\epsilon_a^{3/2}\frac{m_i n_i c^2}{B_p^2}\frac{\partial\mathbf{E}_r}{\partial t}, \tag{25}$$

which corresponds to a neoclassical polarization density of

$$n_{pol} \approx \frac{16}{3\pi\sqrt{2}}\epsilon_a^{3/2}\frac{m_i n_i c^2}{eB_p^2}\frac{\partial^2\phi}{\partial r^2} \tag{26}$$

through the continuity equation. Callen explains this neoclassical current density as "due principally to the spreading of the charge cloud for the trapped ions over the thickness of their banana orbits." Our heuristic derivation follows this description, while also identifying the contribution from the excursion in the toroidal direction as well as the previously known contribution in the radial direction. We note that Hinton and Robertson[50] have studied a closely related issue in a different collisionality regime, and more recent calculations also confirm the scaling in Eq.(25).[43]

In what follows we will see that this heuristic estimate although useful, is only pedagogical and should not be adopted for any serious application. This is due to the difference between the gyrophase-average and bounce-phase-average. Already we have glossed over the fact that θ, the poloidal (and also related to the bounce phase) angle, not only appears in the deviations Δr and $\Delta\alpha$, but also gives the guiding center position along the field line. In gyrokinetics, the gyrophase angle appears only in the Larmor radius deviations and has no relation to the parallel motion. We will discuss this in more detail later.

III. ONE FORM MECHANICS AND LIE PERTURBATION THEORY

In order to derive rigorously the equations of motion that are bounce phase independent, we use the formalism of the Poincaré-Cartan one form.[45,46,53,54] Classical mechanics in this formalism transforms simply under coordinate changes, since a one-form transforms covariantly and the new equations of motion are determined from the one-form, via the principle of least action. In addition, the powerful techniques of Lie perturbation theory[55,44–46] can be employed easily to derive equations of motion which are bounce-phase independent to desired order. Here we present the basics of one-form mechanics and Lie perturbation theory; for greater detail one can refer to the references cited above.

In canonical Cartesian coordinates, the single-particle Poincaré-Cartan one-form is written as

$$\gamma = p_j dq^j - H_c(q^i, p_k)dt, \tag{27}$$

where $j = 1 \ldots 3$, p_j and q^j are canonical momenta and coordinates, respectively, and H_c is the Hamiltonian in canonical coordinates; the summation convention over repeated indices is assumed. A coordinate transform where time is unchanged can be written as $z^\mu = z^\mu(q^i, p_k, t)$ with $\mu = 0 \ldots 6$ and $z^0 = t$; under such a transformation, the Poincaré-Cartan one-form is

$$\begin{aligned} \gamma &= p_j \frac{\partial q^j}{\partial z^\mu} dz^\mu - h(z^\nu) dz^0 \\ &\equiv \gamma_\mu dz^\mu, \end{aligned} \tag{28}$$

where $\gamma_0 \equiv -H_c + p_j \frac{\partial q^j}{\partial z^0}$. Here, the covariant transformation properties are most easily seen. Under another coordinate transformation, $Z^\nu = Z^\nu(z^\mu)$ we have

$$\gamma = \gamma_\mu dz^\mu = \gamma_\mu \frac{\partial z^\mu}{\partial Z^\nu} dZ^\nu \equiv \Gamma_\nu dZ^\nu, \tag{29}$$

and the covariance is manifest. Notice that the coordinate transformations are general transformations and need not be canonical.

The equations of motion can be derived from a variational principle applied to the Poincaré-Cartan one-form. The action associated with a particular one-form is given by

$$S = \int_{t_0}^{t_f} \gamma_\mu \frac{dz^\mu}{dt} dt. \tag{30}$$

Carrying out the minimization of S with respect to variations in the z^μ, we obtain the generalized Euler-Lagrange equations:

$$\left(\frac{\partial \gamma_\mu}{\partial z^\nu} - \frac{\partial \gamma_\nu}{\partial z^\mu} \right) \frac{dz^\mu}{dt} = 0. \tag{31}$$

If we explicitly separate out the time components, we have

$$\hat{\omega}_{ij} \frac{dz^j}{dt} = \frac{\partial h}{\partial z^i} + \frac{\partial \gamma_i}{\partial t} \tag{32}$$

where $\hat{\omega}_{ij} \equiv \partial \gamma_j / \partial z^i - \partial \gamma_i / \partial z^j$ and here, $i, j = 1 \ldots 6$. The tensor $\hat{\omega}_{ij}$ corresponds to the Lagrange brackets, and the inverse $\hat{\omega}_{ij}^{-1}$ are the usual Poisson brackets (in the new coordinates). Thus, knowledge of the Poincaré-Cartan one-form completely determines the equations of motion. Notice that the addition of a perfect derivative dS to the one-form does not change the equations of motion since $\int dS$ does not vary with variations in the path of integration.

So far, we have discussed general transformations, which are usually finite transformations. However, since the bounce phase dependence appears only in small ($\mathcal{O}(\epsilon_B)$ or $\mathcal{O}(\epsilon_\phi)$) quantities, perturbation theory is appropriate for these purposes. Here we use Lie perturbation theory to obtain a coordinate system where the Poincaré-Cartan one-form is bounce phase independent (both in $\gamma_0 = -h$ and the other γ_j's) to desired order. Though the transformation itself is bounce phase dependent, because the transformed γ has no bounce phase dependence, the equations of motion will also be bounce phase independent. (The bounce phase dependence has been removed from the new coordinates and incorporated into the transformation.)

As in usual perturbation theory, we separate the Poincaré-Cartan one-form γ into $\gamma_0+\gamma_1$, where γ_0 is the easily solvable part of the motion and γ_1 is the perturbation. (Note that subscripts can now represent the order in the perturbation expansion, as well as the various components; the usage will be clear from the context.) In our case, only γ_1 contains bounce phase dependence, while the motion specified by γ_0 is bounce phase independent. We seek a Lie transformation of coordinates

$$Z^\mu = \tau z^\mu \tag{33}$$

such that the transformed γ_1 contains no bounce phase dependence. Z^μ and z^μ are the new and old coordinates, respectively, and τ is the Lie transformation. τ can be written as

$$\tau = \ldots \tau_3 \tau_2 \tau_1, \tag{34}$$

where

$$\tau_n = \exp(\epsilon^n L_n), \tag{35}$$

and L_n is an operator with different action on different geometric structures; we will need only its actions on scalars and one-forms. For the transformation $Z^\mu = \tau z^\mu$, a scalar function $f(z^\mu)$ transforms as

$$F = \tau^{-1} f. \tag{36}$$

In this case, L_n acts on $f(z^\mu)$ as

$$(L_n f)(z^\mu) = \left(g_n^\nu(z^\mu) \frac{\partial f}{\partial z^\nu} \right) (z^\mu) \tag{37}$$

where g_n^ν are the generators of the n^{th} order Lie transformation. Notice that the z^μ are only dummy variables; the transformations give the new functional dependences explicitly. Similarly a one-form γ transform as

$$\Gamma = \tau^{-1}\gamma + dS \tag{38}$$

where S is a gauge function which leaves the equations of motion unchanged. For one-forms, L_n acts as

$$(L_n\gamma)_\mu = g_n^\nu \left(\frac{\partial \gamma_\mu}{\partial z^\nu} - \frac{\partial \gamma_\nu}{\partial z^\mu} \right). \tag{39}$$

Expanding the Lie transformation τ to second order, we see that

$$\Gamma_0 = \gamma_0 + dS_0, \tag{40}$$

$$\Gamma_1 = \gamma_1 - L_1\gamma_0 + dS_1, \tag{41}$$

$$\Gamma_2 = \gamma_2 - L_1\gamma_1 + (\frac{1}{2}L_1^2 - L_2)\gamma_0 + dS_2. \tag{42}$$

Thus, by choosing the g_n^μ's and S_n's appropriately we can make our new Poincaré-Cartan one-form bounce phase invariant to desired order.

IV. BOUNCE-KINETIC VLASOV EQUATION

The rigorous derivation of the bounce-kinetic Vlasov equation follows the formalism described in the previous section. Our starting point is the fundamental one-form for the motion of a charged particle in electric and magnetic fields, in canonical Cartesian coordinates. Through a series of transformations the Poincaré-Cartan one-form is brought into a form which can be suitably averaged. The equilibrium part of the one-form with only a static magnetic field will be considered first; the knowledge of the unperturbed particle motion determines the manner in which the perturbation theory is applied. Self-consistency of the perturbed electrostatic field is enforced by the accompanying Poisson equation.

The equilibrium fundamental one-form in canonical coordinates is

$$\gamma_0 = p_j dq^j - h_c dt, \tag{43}$$

where $h_c = (\mathbf{p} - e\mathbf{A}/c)^2/2m$ and $j = 1 \ldots 3$. After transforming to velocity space (instead of momentum space) and making the guiding center transformation (for more details, see Refs. 4 and 33), we have

$$\gamma_0 = \left[\frac{e}{c}\mathbf{A}_0(\mathbf{X}) + mv_\parallel \mathbf{b}(\mathbf{X})\right] \cdot d\mathbf{X} + \frac{mc}{e}\mu d\theta - \left[\mu B(\mathbf{X}) + \frac{1}{2}mv_\parallel^2\right] dt, \tag{44}$$

where $\mathbf{X}$ is the guiding center position, $\mu = mv_\perp^2/2B$ is the magnetic moment, and $v_\parallel$ and $v_\perp$ are the velocities parallel and perpendicular to the magnetic field, respectively. Here the bounce motion in a non-uniform magnetic field is apparent in the last term: the conservation of μ and the total energy requires $v_\parallel$ to be zero for large enough $B(\mathbf{X})$. To make the bounce motion of trapped particles readily apparent, the Poincaré-Cartan one-form is transformed into flux and action-angle coordinates in the bounce motion.[47] This is written in two steps to make the physical motion more apparent; also, the gyrophase dependence is dropped since we are not interested in the bounce-averaged gyrophase motion. (In fact, throughout the derivation the Larmor radius is assumed sufficiently small compared to the bounce deviation that it can be ignored.) Letting $\mathbf{B}(\mathbf{X}) = \nabla\alpha \times \nabla\beta$, choosing the gauge so that $\mathbf{A}(\mathbf{X}) = \alpha\nabla\beta$, and denoting the distance along the field line by s, the fundamental one-form is

$$\gamma_0 = \frac{e}{c}\alpha d\beta + mv_\parallel ds - \left[\mu B(\alpha, \beta, s) + \frac{1}{2}mv_\parallel^2\right] dt. \tag{45}$$

At this point, we introduce the notation $y_1 = \beta$ and $y_2 = \alpha$ and let a and b be indices which take on the values 1 to 2. The equilibrium one-form has bounce phase dependence, but only in a quantity $\mathcal{O}(\epsilon_B)$ compared to the other terms. The transformation to action-angle coordinates which makes the equilibrium one-form bounce phase independent is more complicated, and the results will only be summarized (see Ref. 41 for details). The motivation for this particular choice of variables comes from the lowest order motion of the guiding center along a field line; if α, β are held constant, the lowest order motion is given by

$$\frac{ds}{dt} = v_\parallel \tag{46}$$

$$m\frac{dv_\parallel}{dt} = -\mu\frac{\partial B}{\partial s}(\alpha, \beta, s); \tag{47}$$

these are the equations of motion of an oscillator, and so one can define action and angle coordinates for this bounce motion. For the lowest order motion, we let

$$I(K_0, \alpha, \beta) = \frac{1}{\pi}\int_{s_0}^{s_1} \left[2m(K_0 - \mu B)\right]^{1/2} ds' \tag{48}$$

$$\psi(s, v_\parallel, K_0, \alpha, \beta) = \pi + sgn(v_\parallel)\omega_B \int_{s_0}^{s} \frac{ds'}{\left[2m(K_0 - \mu B)\right]^{1/2}} \tag{49}$$

where K_0 is the numerical value of the particle energy, and $\omega_B(I, \alpha, \beta)$, the bounce frequency, is defined as $\partial h_0/\partial I(\mathbf{y}, I)$, since the total energy h_0 can be written in terms of I. Note that these expressions are only for the lowest order bounce motion, where we have assumed the guiding center is fixed to a given field line. The "true" action and angle variables are different from these expressions by terms of order ϵ_B. The derivation of these terms will not be presented here (see Ref. 41); we present only the final equilibrium one-form and the explicit coordinate transformations. After the application of a noncanonical Lie perturbation transformation, we have:

$$\gamma_0 = \frac{e}{c}Y_2 dY_1 + J d\Psi - H(Y_2, Y_1, J)dt, \tag{50}$$

where

$$Y_a = y_a - \eta_{ab}F_b(\mathbf{y}, I, \psi), \tag{51}$$

$$J = I + \frac{1}{\omega_B}\left(\eta_{ab}F_b\frac{\partial h_0}{\partial y_a}\right), \tag{52}$$

$$\Psi = \psi + g_1^\psi(\mathbf{y}, I, \psi), \tag{53}$$

with $\eta_{11} = \eta_{22} = 0$, $\eta_{12} = -\eta_{21} = 1$, and

$$F_a(\mathbf{y}, I, \psi) = \frac{mc}{e} \int_0^I dI' \left(\frac{\partial}{\partial I'} \left(v_\parallel \mathbf{b} \cdot \frac{\partial \mathbf{X}}{\partial y_a} \right) - \frac{\partial}{\partial y_a} \left(v_\parallel \frac{\partial s}{\partial I'} \right) \right); \tag{54}$$

the explicit form for g_1^ψ will not be needed. F_2 and F_1 correspond physically to the deviations from the bounce center radial (β) or field line (α) position, respectively, and $\mathbf{Y}$ gives the bounce center position.

With this expression for the bounce phase independent equilibrium one-form, we can now carry out the Lie perturbation analysis for the electrostatic fluctuation. The above expression is valid to second order in ϵ_B, and the perturbation analysis will be expanded to second order in ϵ_ϕ. Adding the electric field perturbation to the equilibrium one-form, we have

$$\gamma = \frac{e}{c} Y_2 dY_1 + J d\Psi - H_0(\mathbf{Y}, J) dt - e\phi(\mathbf{y}, s) dt. \tag{55}$$

Throughout the derivation, ϕ is written as a function of $(\mathbf{y}, s)$. Thus, in $(\mathbf{Y}, J, \Psi)$ coordinates,

$$\phi(\mathbf{y}, s) = \phi\left(Y_a + \eta_{ab} F_b(\mathbf{Y}, J, \Psi), s(J, \Psi)\right). \tag{56}$$

In order to have a bounce phase independent one-form, to first order in ϵ_ϕ we seek a transformation which brings ϕ into $\langle\phi\rangle$, where

$$\langle\phi\rangle(\mathbf{Y}, J) = \frac{1}{2\pi} \oint d\Psi \phi(Y_a + \eta_{ab} F_b, s(J, \Psi)). \tag{57}$$

That is, we seek S_1 and g_1^ν so that $-L_1\gamma_0 + dS_1 = e(\phi - \langle\phi\rangle)dt$ (see Eq. (41)). The determination of the generators and the gauge function is a linear system of five equations for five unknowns and thus is solvable. (In full generality, this would be an 8×8 system, but we have restricted ourselves to transformations which do not affect time and have ignored the gyrophase action and angle variables.) The explicit form for the generators, which is necessary for the construction of the Poisson equation and the polarization density, can be determined iteratively in the longwavelength limit, $\epsilon_k \sim \omega/\omega_B \sim k_\perp \Lambda_B \ll 1$. In this case, the first order generators are

$$
\begin{aligned}
g_1^J &= g_{10}^J + \epsilon_k g_{11}^J + \ldots \\
&= \frac{e\tilde{\phi}}{\omega_B} + \frac{1}{\omega_B}\left(-\frac{e}{\omega_B}\frac{\partial\tilde{\Phi}}{\partial t} + \eta_{ab}\frac{c}{e}\frac{\partial}{\partial Y_b}\left(\frac{e\tilde{\Phi}}{\omega_B}\right)\frac{\partial H_0}{\partial Y_a}\right) + \ldots \qquad (58)\\
g_1^a &= g_{10}^a + g_{11}^a \ldots \\
&= -\eta_{ab}\frac{c}{e}\frac{\partial}{\partial Y_b}\left(\frac{e\tilde{\Phi}}{\omega_B}\right) \qquad (59)\\
g_1^\Psi &= g_{10}^\Psi + g_{11}^\Psi + \ldots \\
&= -\frac{\partial}{\partial J}\left(\frac{e\tilde{\Phi}}{\omega_B}\right). \qquad (60)
\end{aligned}
$$

Here, $\tilde{\phi} \equiv \phi - \langle\phi\rangle$, and $\tilde{\Phi} \equiv \int d\Psi'\tilde{\phi}$; we have displayed only terms in ϵ_k necessary to obtain a final system good to $\mathcal{O}(\epsilon_k^2)$.

For second order, S_2 and g_2^ν are similarly determined. To lowest order in ϵ_k,

$$
\Gamma_{2t} = \frac{e^2}{2}\left\langle -\frac{c}{e}\eta_{ab}\left(\frac{\partial}{\partial\overline{Y_b}}\frac{1}{\omega_B}\int^{\overline{\Psi}}\tilde{\phi}d\overline{\Psi}'\right)\frac{\partial\tilde{\phi}}{\partial\overline{Y_a}} + \frac{\partial}{\partial\overline{J}}\frac{\tilde{\phi}^2}{\omega_B}\right\rangle, \qquad (61)
$$

where overbars are used for the new, bounce-averaged coordinates. Defining the effective potential as

$$
\phi_{\text{eff}}(\overline{\mathbf{Y}},\overline{J}) \equiv \langle\phi\rangle + \frac{e}{2}\left\langle\frac{c}{e}\eta_{ab}\left(\frac{\partial}{\partial\overline{Y_b}}\frac{1}{\omega_B}\int^{\overline{\Psi}}\tilde{\phi}d\overline{\Psi}'\right)\frac{\partial\tilde{\phi}}{\partial\overline{Y_a}} - \frac{\partial}{\partial\overline{J}}\frac{\tilde{\phi}^2}{\omega_B}\right\rangle, \qquad (62)
$$

the bounce-averaged fundamental one-form is

$$
\Gamma = \frac{e}{c}\overline{Y_2}d\overline{Y_1} + \overline{J}d\overline{\Psi} - H_0(\overline{\mathbf{Y}},\overline{J})dt - e\phi_{\text{eff}}(\overline{\mathbf{Y}},\overline{J})dt. \qquad (63)
$$

$H_0(\overline{\mathbf{Y}},\overline{J})$ has the same functional form as the unaveraged Hamiltonian but is in terms of the new averaged coordinates. From the fundamental one-form Poisson brackets of the bounce-averaged coordinate system are straightforwardly determined; the new coordinates are canonical (up to a normalization):

$$
\{\overline{Y_1},\overline{Y_2}\} = \frac{c}{e}, \qquad (64)
$$

$$
\{\overline{\Psi},\overline{J}\} = 1; \qquad (65)
$$

all other Poisson brackets are zero. Using Eq. (32), the bounce-averaged equations of motion are

$$\frac{d\overline{Y_1}}{dt} = \frac{c}{e}\left(\frac{\partial H_0}{\partial \overline{Y_2}} + e\frac{\partial \phi_{\text{eff}}}{\partial \overline{Y_2}}\right) \tag{66}$$

$$\frac{d\overline{Y_2}}{dt} = -\frac{c}{e}\left(\frac{\partial H_0}{\partial \overline{Y_1}} - e\frac{\partial \phi_{\text{eff}}}{\partial \overline{Y_1}}\right) \tag{67}$$

$$\frac{d\overline{\Psi}}{dt} = \frac{\partial H_0}{\partial \overline{J}} + e\frac{\partial \phi_{\text{eff}}}{\partial \overline{J}} \tag{68}$$

$$\frac{d\overline{J}}{dt} = 0. \tag{69}$$

The drift equations of motion presented in Sec. 2 are a special case of these equations. Eqs. (66) and (67) express the motion in the radial and α directions, respectively. For an axisymmetric tokamak equilibrium, the bounce-averaged radial velocity is zero because $\partial H_0/\partial \overline{Y_2}$ is zero; on the other hand, $\partial H_0/\partial \overline{Y_1}$ is non-zero and represents the precessional motion in the toroidal direction. In both equations, the bounce averaged radial and α-directed electric fields give rise to bounce-averaged motion. Eq. (68) evolves the bounce phase angle, while Eq. (69) states that $\overline{J}$ is the second order approximation to the true adiabatic invariant associated with trapped particle motion.

Because the Vlasov equation is covariant,[46] its form is easily determined via

$$\frac{\partial f}{\partial z^\mu}\frac{dz^\mu}{dt} = \frac{\partial F}{\partial Z^\mu}\frac{dZ^\mu}{dt}, \tag{70}$$

where F is the distribution function written as a function of the barred coordinates $(\overline{\mathbf{Y}}, \overline{J}, \overline{\mu}, t)$ but has no $\overline{\Psi}$ dependence.[3] Thus the bounce-averaged Vlasov equation is simply

$$\frac{\partial F}{\partial t} + \frac{d\overline{Y_1}}{dt}\frac{\partial F}{\partial \overline{Y_1}} + \frac{d\overline{Y_2}}{dt}\frac{\partial F}{\partial \overline{Y_2}} = 0. \tag{71}$$

V. BOUNCE-KINETIC POISSON EQUATION AND NEOCLASSICAL POLARIZATION DENSITY

Having derived the equations of motion for given fields, we must now derive the associated Poisson equation. In dealing with collective fluctuation phenomena, the bounce-kinetic Poisson equation is as important as the bounce-kinetic Vlasov equation because self-consistency is required. The bounce-averaged Poisson equation relies upon the correct determination of the trapped particle density. Following Ref. 3 the general expression for the particle density from the distribution function is

$$n(\mathbf{x},t) \equiv \int d^3\mathbf{x}' d^3\mathbf{v}\,\delta(\mathbf{x}-\mathbf{x}')f(\mathbf{x}',\mathbf{v},t). \tag{72}$$

Now remains the straight-forward though tedious process of transforming the integral, δ-function, and distribution function into the bounce-averaged flux and action-angle coordinates as defined above. The details of this calculation can be found in the appendix. The final trapped particle density in the bounce-averaged coordinates is

$$\begin{aligned} n(\beta,\alpha,s,t) = &\int' \frac{B\omega_B}{m^2|v_\parallel|} d\overline{Y_1}d\overline{Y_2}d\overline{\Psi}d\overline{J}d\overline{\mu}d\overline{\theta}\delta(y_a - \overline{Y_a} - \eta_{ab}\overline{F_b})\delta(h(s,\overline{J}) - \overline{\Psi} + g_1^\psi) \\ &\times \left(F(\overline{\mathbf{Y}},\overline{J},\overline{\mu},t) + g_1^J \frac{\partial F}{\partial \overline{J}} + g_1^a \frac{\partial F}{\partial \overline{Y_a}} \right), \end{aligned} \tag{73}$$

where the prime indicates integration over the trapped particles only, and the first order generators are given by Eqns. (58) and (59). (Since F has no $\overline{\Psi}$ dependence the first order generator g_1^ψ plays no role in determination of the density.) This expression is valid to $\mathcal{O}(\epsilon_B)$, $\mathcal{O}(\epsilon_\phi)$, and $\mathcal{O}(\epsilon_k^2)$. The key difference between gyrokinetics and bounce-kinetics appears in the δ-function of the bounce phase angle. In gyrokinetics, the field line direction, s is independent of the gyrophase angle, θ, whereas in bounce-kinetics, s directly depends on the bounce phase angle ψ. The θ integration in gyrokinetics averages over the gyrophase, but here, because of the δ-function, the $\overline{\Psi}$ integration evaluates the integrand at the $\overline{\Psi}$ corresponding to the given field line position and bounce action. The "bounce averaging" in the expression for the density is only an average in the sense that it averages over all $\overline{\Psi}$'s via the integration over the possible values of the bounce action at a given field line position, s.

Eqs. (66)–(69), (71), and (73) are the self-consistent set of equations which can be used to model low frequency phenomena associated with trapped particle behavior in arbitrary magnetic geometries that satisfy the assumed orderings. For applications, the specialization to tokamak geometry is more useful. In order to keep the expressions analytically tractable, the deeply trapped particle limit is assumed, as well as ($\epsilon_k \sim k_\perp \Lambda_B \ll 1$). In this case, lowest order flux and action-angle coordinates are given by

$$\beta \equiv \psi_p(r) \tag{74}$$

$$\alpha \equiv \zeta - q(r)\theta \tag{75}$$

$$\psi \approx \pi + \mathrm{sgn}(v_\parallel)\left[\arcsin\left(\frac{\sin\frac{\theta}{2}}{\kappa}\right) + \frac{\pi}{2}\right] \tag{76}$$

$$I \approx 2qR_0\sqrt{m\epsilon_a\mu B_0}\kappa^2, \tag{77}$$

where $\psi_p(r)$ is the poloidal flux function, and κ is the same pitch angle parameter introduced in Sec. 2,

$$\kappa^2 = \frac{K_0 - \mu B_0(1-\epsilon_a)}{2\epsilon_a\mu B_0(1-\epsilon_a)}, \tag{78}$$

where K_0 is the numerical value of the total particle energy. The Hamiltonian and bounce frequency are given by

$$H_0(\beta, I, \mu) \approx \mu B_0(1-\epsilon_a) + \frac{I\sqrt{\epsilon_a\mu B_0}}{qR_0\sqrt{m}}, \tag{79}$$

$$\omega_B \approx \frac{\sqrt{\epsilon_a\mu B_0}}{qR_0\sqrt{m}}. \tag{80}$$

Note that H_0 has β dependence arising from ϵ_a and q, but is independent of α. Applying the necessary transformations described above, the final equations of motion are

$$\frac{d\overline{Y_1}}{dt} = e\frac{\partial\phi_{\text{eff}}}{\partial\overline{Y_2}} \tag{81}$$

$$\frac{d\overline{Y_2}}{dt} = -\frac{c}{e}\left(\frac{\partial H_0}{\partial\overline{Y_1}} - e\frac{\partial\phi_{\text{eff}}}{\partial\overline{Y_1}}\right) \tag{82}$$

$$\frac{d\overline{\Psi}}{dt} = \omega_B(\overline{Y_b}, \overline{J}) + e\frac{\partial\phi_{\text{eff}}}{\partial\overline{J}} \tag{83}$$

$$\frac{d\overline{J}}{dt} = 0, \tag{84}$$

where H_0 and ω_B have the same functional form as in Eqs. (79) and (80), though their arguments are the bounce-averaged variables, rather than the lowest order variables.

As for the Poisson equation, keeping terms to $\mathcal{O}(\epsilon_k^2)$, Eq. (73) reduces to

$$n_{i,\text{trapped}}(\beta, \alpha, s, t) =$$

$$\hat{N}_{i,\text{trapped}}(\beta, \alpha, s, t) + \sqrt{2}\frac{mc^2}{e}\epsilon_a^{3/2}R_0^2(\kappa_m^2 - u)^{1/2}N_i$$

$$
\begin{aligned}
&\times\left[\frac{\partial^2\phi}{\partial\beta^2}\left(\frac{5}{4}(\kappa_m^2-u)+\frac{3}{4}u+\frac{1}{2\epsilon_a}u^{1/2}q\frac{1}{N_i}\frac{\partial N_i}{\partial\alpha}\right)\right.\\
&\quad+\frac{\partial^2\phi}{\partial\alpha^2}\left(\frac{1}{2\epsilon_a}\left(u-\frac{1}{3}(\kappa_m^2-u)\right)\sigma q\frac{1}{N_i}\frac{\partial N_i}{\partial\beta}+\left(\frac{3}{8}u^2+\frac{5}{4}u(\kappa_m^2-u)+\frac{3}{40}(\kappa_m^2-u)^2\right)\sigma^2\right.\\
&\qquad\left.+\left(-\frac{3}{4}u+\frac{3}{2}u^2+\frac{1}{4}(\kappa_m^2-u)-\frac{3}{10}(\kappa_m^2-u)^2\right)\sigma q\frac{1}{T_i}\frac{\partial T_i}{\partial\beta}\right)\\
&\quad+\frac{\partial^2\phi}{\partial\alpha\partial\beta}\left(-2u^{1/2}(\kappa_m^2-u)\sigma-\frac{2}{\epsilon_a}u^{1/2}q\frac{1}{N_i}\frac{\partial N_i}{\partial\beta}+\frac{1}{6\epsilon_a}(\kappa_m^2-u)\sigma q\frac{1}{N_i}\frac{\partial N_i}{\partial\alpha}\right.\\
&\qquad\left.+u^{1/2}\left(3-2\left((\kappa_m^2-u)+3u\right)\right)q\frac{1}{T_i}\frac{\partial T_i}{\partial\beta}\right)\\
&\quad+\frac{\partial\phi}{\partial\beta}\left(2(\kappa_m^2-u)\left(\frac{1}{N_i}\frac{\partial N_i}{\partial\beta}-\frac{\sigma}{q}\right)-2u^{1/2}(\kappa_m^2-u)\sigma\frac{1}{N_i}\frac{\partial N_i}{\partial\alpha}+\frac{1}{2\epsilon_a}u^{1/2}\frac{\partial q}{\partial\beta}\frac{1}{N_i}\frac{\partial N_i}{\partial\alpha}\right)\\
&\quad+\frac{\partial\phi}{\partial\alpha}\left(-2u^{1/2}(\kappa_m^2-u)\left(\frac{1}{N_i}\frac{\partial N_i}{\partial\beta}-\frac{\sigma}{q}\right)+2u(\kappa^2-u)\sigma^2\frac{1}{N_i}\frac{\partial N_i}{\partial\alpha}\right.\\
&\qquad\left.-\frac{1}{\epsilon_a}\left(u\frac{\partial}{\partial\beta}(q\sigma)-\frac{1}{2}\left(u+\frac{1}{3}(\kappa_m^2-u)\right)q\sqrt{\epsilon_a}\frac{\partial}{\partial\beta}\left(\frac{\sigma}{\sqrt{\epsilon_a}}\right)\right)\right)\\
&\quad\left.+\frac{\partial^2\phi}{\partial t\partial\beta}\frac{eq}{c\epsilon_aT_i}u^{1/2}-\frac{\partial^2\phi}{\partial t\partial\alpha}\frac{2e\sigma q}{c\epsilon_aT_i}\left(u-\frac{1}{3}(\kappa_m^2-u)\right)\right]
\end{aligned}\tag{85}
$$

where $\hat{N}_i$, the bounce-averaged banana center density, is defined as

$$
\begin{aligned}
\hat{N}_i(\beta,\alpha,s,t)=\int'\frac{B\omega_B}{m^2|v_\parallel|}d\overline{Y_1}d\overline{Y_2}d\overline{\Psi}d\overline{J}d\overline{\mu}d\overline{\theta}\delta(y_a-\overline{Y_a}-\eta_{ab}\overline{F_b})\delta(h(s,\overline{J})-\overline{\Psi}+g_1^{\psi})\\
\times\left(F(\overline{\mathbf{Y}},\overline{J},\overline{\mu},t),\right)
\end{aligned}\tag{86}
$$

and N_i is the density of trapped particle banana centers, that is,

$$
F(\overline{\mathbf{Y}},\overline{J},\overline{\mu},t)\equiv\frac{N_i(\overline{\mathbf{Y}},t)}{(\pi v_{th}^2)^{3/2}}\exp\left(-H_0/T_i(\overline{Y_1})\right);\tag{87}
$$

u and σ are defined as

$$
\begin{aligned}
u&\equiv\sin^2\left(\frac{s}{2qR_0}\right)\\
\sigma&\equiv\frac{\partial q}{\partial\beta}-\frac{q}{2\epsilon_a}\frac{\partial\epsilon_a}{\partial\beta};
\end{aligned}\tag{88}
$$

κ_m^2 corresponds to the deeply trapped particle cutoff in pitch angle space. Due to the approximations made in Eqs. (74)–(80), our results are rigorously valid only for deeply trapped particles with $u\le\kappa_m^2\ll1$; $\kappa_m^2=1$ corresponds to the trapped-passing boundary.

The details of the calculation are given in the Appendix. The form for the trapped ion density in Eq. (85) has close similarity to the analogous gyrokinetic ion density.[3] The energy invariant for the bounce kinetic system is

$$\int' H_0 F_{i,\text{banana center}} d^6Z + \int' \frac{1}{2} g_1^j \frac{\partial}{\partial Z^j}\left(g_1^i \frac{\partial H_0}{\partial Z^i}\right) d^6Z + \int \frac{m_i v^2}{2} f_{i,\text{passing}} d^6z \\ + \int \frac{m_e v^2}{2} f_e d^6z + \int \frac{|\mathbf{E}|^2}{8\pi} d^3x = \text{constant}. \tag{89}$$

The self-consistent determination of the fluctuating potential is given by

$$\nabla^2\phi = -4\pi e(n_{i,\text{trapped}} + n_{i,\text{passing}} - n_e). \tag{90}$$

Assuming quasi-neutrality, the Poisson equation reduces to

$$n_{i,\text{trapped}} + n_{i,\text{passing}} - n_e \approx 0, \tag{91}$$

which is a useful form for simulation purposes; the response of the passing ions can be obtained from gyrokinetics, although the adiabatic response is a very good approximation for the low frequency range we are considering. (The bounce-averaging could also apply to the trapped electrons,[20] though because of the electron mass, their bounce radii are considerably smaller than those of the trapped ions.)

The rigorous form for the nonlinear neoclassical polarization density is given by Eq. (85); it is the difference between the real trapped particle density and the bounce-averaged banana center density. Several features arise from the rigorous calculation that were not apparent in the heuristic estimate. First, the polarization density has explicit field line dependence. This is a natural consequence of the finite poloidal excursion of trapped particles, and has not been addressed in previous studies. Also, the heuristic estimate as presented in Section II incorrectly eliminates this salient feature via the ad-hoc averaging procedure. The polarization density also has nonlinear terms proportional to ϕ^2 because of the ϕ dependence in the fluctuating part of N_i. Last, the rigorous calculation includes the effects of equilibrium density gradients and cross terms, which previously averaged to zero; these terms are necessary for proper energy conservation.

Finally, we note that the axisymmetric limit $\frac{\partial}{\partial\alpha} = 0$ of Eq.(85) can be used for studying the long term behavior of fluctuation driven $\mathbf{E}\times\mathbf{B}$ flow. In particular, the aforementioned field line dependence will provide useful insights into the recent gyrokinetic simulation result[31] which shows that a significant $m = 0$ component of $\mathbf{E}\times\mathbf{B}$ flow can be driven by $m \neq 0$ components of turbulence.

VI. SUMMARY AND DISCUSSION

In this work, we have derived the nonlinear electrostatic bounce-averaged kinetic equations via phase-space Lagrangian Lie-perturbation theory. This symplectic derivation ensures the preservation of the Hamiltonian structure and conservation laws. This new bounce-averaged kinetic formalism provides a firm theoretical foundation for description of the low frequency large scale fluctuations such as the trapped ion mode, turbulence driven $\mathbf{E}\times\mathbf{B}$ flow, and convective cells often observed in tokamak plasmas.

Full banana orbit width effects are retained in both the bounce-averaged Vlasov equation and Poisson equation. In the bounce-kinetic Poisson equation, the general form of the neoclassical polarization density term is obtained, and its relevance to the long term behavior of turbulence driven $\mathbf{E}\times\mathbf{B}$ flow is discussed. We find that the neoclassical polarization density arises from the difference between the real trapped particle density and the bounce-averaged banana center density across the magnetic field lines. We have identified the contribution from the toroidal excursion in addition to the previously known contribution from the radial excursion. A nonlinearity associated with this new term plays an important role in the collisionless trapped ion turbulence model.[37]

Both similarities and differences between the bounce-averaged kinetic equations and the gyrokinetic equations are discussed in this work. The formalism presented in this paper should be useful for future bounce-kinetic particle-in-cell simulations of trapped particle modes and the generalization of present nonlinear bounce-averaged gyrofluid equations.[56] Since there is accumulating evidence that the $\mathbf{E}\times\mathbf{B}$ shear suppression of turbulence[57–59] plays an essential role in enhancing tokamak core confinement, it is important to generalize our formalism by including the equilibrium $\mathbf{E}\times\mathbf{B}$ shear effects.[60–68] Fluctuations with long radial correlation length are especially susceptible to the $\mathbf{E}\times\mathbf{B}$ shear suppression. Following the recent advances in the gyrokinetic formalism,[69] such $\mathbf{E}\times\mathbf{B}$ shear effects can be systematically included in our formalism.

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APPENDIX: DENSITY CALCULATIONS

In this appendix, the form for the trapped particle density in arbitrary geometries will be derived and then specialized to the case of a tokamak (with further qualifications discussed below). The breakdown of the analogy between bounce-kinetics and gyrokinetics will become apparent in the course of the derivation. The starting point is Eq. (72),

$$n(\mathbf{x},t)\equiv\int d^3\mathbf{x}'d^3\mathbf{v}\delta(\mathbf{x}-\mathbf{x}')f(\mathbf{x}',\mathbf{v},t). \tag{A1}$$

Assuming the equivalence of the real particle position and the guiding center position, the distribution function moment transforms to

$$n(\mathbf{X},t)=\int\frac{B^*}{m}d^3\mathbf{X}'dv_\parallel d\mu d\theta\delta(\mathbf{X}-\mathbf{X}')f_{\text{g.c.}}(\mathbf{X}',v_\parallel,\mu,t), \tag{A2}$$

where $B^*=B+(mc/e)v_\parallel\hat{b}\cdot\nabla\times\hat{b}$ is the Jacobian of the six-dimensional guiding center transformation. Instead of continuing to express the density in terms of the Cartesian position, the derivation is simplified by considering it as a function of the field line coordinates. Thus, one has

$$
\begin{aligned}
n(\beta,\alpha,s,t) &= \int \frac{B^*}{m}\left|\frac{\partial^3\mathbf{X}'}{\partial\beta'\partial\alpha'\partial s}\right| d\beta' d\alpha' ds' dv_\parallel d\mu d\theta\,\delta(\mathbf{X}'(\beta',\alpha',s') - \mathbf{X}(\beta,\alpha,s)) \\
&\qquad \times f_{\text{flux}}(\beta',\alpha',s',v_\parallel,\mu,t) \\
&= \int \frac{B^*}{m} d\beta' d\alpha' ds' dv_\parallel d\mu d\theta\,\delta(\beta'-\beta)\delta(\alpha'-\alpha)\delta(s'-s) f_{\text{flux}}(\beta',\alpha',s',v_\parallel,\mu,t). \quad \text{(A3)}
\end{aligned}
$$

The previous expressions are valid for all particles; for trapped particles the lowest order action-angle variables are defined above, giving

$$
\begin{aligned}
&n_{\text{trapped}}(\beta,\alpha,s,t) \\
&= \int' \frac{B^*}{m^2} d\beta' d\alpha' d\psi dI d\mu d\theta\,\delta(\beta'-\beta)\delta(\alpha'-\alpha)\delta(s'(\psi,I)-s) f_{\text{flux,a-a}}(\beta',\alpha',\psi,I,\mu,t). \\
&= \int' \frac{B^*}{m^2} d\beta' d\alpha' d\psi dI d\mu d\theta\,\delta(\beta'-\beta)\delta(\alpha'-\alpha)\frac{\delta(\psi - h(s,I))}{|\partial s'/\partial\psi|} f_{\text{flux,a-a}}(\beta',\alpha',\psi,I,\mu,t), \quad \text{(A4)}
\end{aligned}
$$

where h expresses the relationship between (s, I) and ψ, and the integration is over trapped particles only. Here the difference between the bounce-averaging and gyroaveraging is readily apparent. Whereas the integral over $d\theta$ plays no role in the δ-functions in gyrokinetics and so averages the integrand over the gyrophase angle, the $d\psi$ integral and δ-function together pick out the particular value of ψ in terms of I and the given field line position, s. We now transform to the true action-angle coordinates following Littlejohn,[46]

$$
\begin{aligned}
n_{\text{trapped}}(\beta,\alpha,s,t) &= \int' \frac{B}{m^2} dY_1 dY_2 d\Psi dJ d\mu d\theta\,\delta(y_a - Y_a - \eta_{ab}F_b) \\
&\qquad \times \frac{\delta(h(s,J) - \Psi + g_1^\psi)}{|\partial s/\partial\Psi|} f_{\text{true}}(\mathbf{Y},\Psi,J,\mu,t); \quad \text{(A5)}
\end{aligned}
$$

g_1^ψ is a generator of the noncanonical Lie transformation of the equilibrium one form and not a generator of the canonical fluctuation average transformation. The final step is to write the distribution function in terms of the bounce-averaged coordinates; their relationship is given by Eq. (36). Letting F be the distribution function in bounced averaged coordinates, we have

$$
\begin{aligned}
f_{\text{true}} &= \tau F \\
&\approx F + g_1^J \frac{\partial F}{\partial J} + g_1^a \frac{\partial F}{\partial Y_a}. \quad \text{(A6)}
\end{aligned}
$$

Finally, in terms of bounce-averaged variables, the trapped particle density is

$$n_{\text{trapped}}(\beta,\alpha,s,t)=\int' \frac{B\omega_B}{m^2|v_\parallel|}d\overline{Y_1}d\overline{Y_2}d\overline{\Psi}d\overline{J}d\overline{\mu}d\overline{\theta}\delta(y_a-\overline{Y_a}-\eta_{ab}\overline{F_b})\delta(h(s,\overline{J})-\overline{\Psi}+g_1^{\psi})$$
$$\times\left(F(\overline{\mathbf{Y}},\overline{J},\overline{\mu},t)+g_1^J\frac{\partial F}{\partial \overline{J}}+g_1^a\frac{\partial F}{\partial \overline{Y_a}}\right). \tag{A7}$$

This expression for the trapped particle density is valid to $\mathcal{O}(\epsilon_\phi)$ and is not yet specialized to tokamak geometry. Keeping terms of $\mathcal{O}(\epsilon_k^2)\sim(k_\perp\Lambda_B)^2$, the trapped particle density reduces to

$$\begin{aligned}
n_{\text{trapped}}(\beta,\alpha,s,t)=\hat{N}_i+\int' &\frac{Be}{m^2|v_\parallel|}d\overline{J}d\overline{\mu}d\overline{\theta}\\
&\times\Bigg[\left(-(F_1^2+\langle F_1^2\rangle)\frac{\partial^2\phi}{\partial\alpha^2}-(F_2^2+\langle F_2^2\rangle)\frac{\partial^2\phi}{\partial\beta^2}+2(F_1F_2+\langle F_1F_2\rangle)\frac{\partial^2\phi}{\partial\beta\partial\alpha}\right)\frac{\partial F}{\partial\overline{J}}\\
&+2\left[-F_1^2\frac{\partial\phi}{\partial\alpha}\frac{\partial^2 F}{\partial\alpha\partial\overline{J}}-F_2^2\frac{\partial\phi}{\partial\beta}\frac{\partial^2 F}{\partial\beta\partial\overline{J}}+F_1F_2\frac{\partial\phi}{\partial\beta}\frac{\partial F}{\partial\alpha\partial\overline{J}}+F_1F_2\frac{\partial\phi}{\partial\alpha}\frac{\partial F}{\partial\beta\partial\overline{J}}\right]\\
&+2\Bigg[\frac{c}{e}\Bigg(\frac{\partial H_0}{\partial\beta}\frac{\partial}{\partial\alpha}\left(\frac{1}{\omega_B}\int^{\overline{\Psi}}d\overline{\Psi}'F_2\frac{\partial\phi}{\partial\beta}\right)-\frac{\partial H_0}{\partial\beta}\frac{\partial}{\partial\alpha}\left(\frac{1}{\omega_B}\int^{\overline{\Psi}}d\overline{\Psi}'F_1\frac{\partial\phi}{\partial\alpha}\right)\\
&-\frac{\partial H_0}{\partial\alpha}\frac{\partial}{\partial\beta}\left(\frac{1}{\omega_B}\int^{\overline{\Psi}}d\overline{\Psi}'F_2\frac{\partial\phi}{\partial\beta}\right)+\frac{\partial H_0}{\partial\alpha}\frac{\partial}{\partial\beta}\left(\frac{1}{\omega_B}\int^{\overline{\Psi}}d\overline{\Psi}'F_1\frac{\partial\phi}{\partial\alpha}\right)\Bigg)\\
&-\frac{1}{\omega_B}\left(\int^{\overline{\Psi}}d\overline{\Psi}'F_2\frac{\partial}{\partial t}\frac{\partial\phi}{\partial\beta}-\int^{\overline{\Psi}}d\overline{\Psi}'F_1\frac{\partial}{\partial t}\frac{\partial\phi}{\partial\alpha}\right)\Bigg]\frac{\partial F}{\partial\overline{J}}\\
&-2\frac{c\omega_B}{e}\Bigg[\frac{\partial F}{\partial\beta}\frac{\partial}{\partial\alpha}\left(\frac{1}{\omega_B}\frac{\partial\phi}{\partial\beta}\int^{\overline{\Psi}}d\overline{\Psi}'F_2\right)-\frac{\partial F}{\partial\beta}\frac{\partial}{\partial\alpha}\left(\frac{1}{\omega_B}\frac{\partial\phi}{\partial\alpha}\int^{\overline{\Psi}}d\overline{\Psi}'F_1\right)\\
&-\frac{\partial F}{\partial\alpha}\frac{\partial}{\partial\beta}\left(\frac{1}{\omega_B}\frac{\partial\phi}{\partial\beta}\int^{\overline{\Psi}}d\overline{\Psi}'F_2\right)+\frac{\partial F}{\partial\alpha}\frac{\partial}{\partial\beta}\left(\frac{1}{\omega_B}\frac{\partial}{\partial\alpha}\int^{\overline{\Psi}}d\overline{\Psi}'\right)\Bigg]\Bigg]
\end{aligned} \tag{A8}$$

after integration over the δ-functions; all real space arguments are now dependent on β,α, and s because of these integrations; the $\overline{\Psi}'$ integrations are evaluated at $\overline{\Psi}(s,\overline{J})$. Also, in this step we have used the fact that the bounce deviations F_a are odd functions of the bounce phase angle ψ. For given s and $\overline{J}$, the δ-function integration over $\overline{\Psi}$ gives two possible values for ψ, depending on the sign of $v_\parallel$; because of the oddness and periodicity of F_a, terms of $\mathcal{O}(k_\perp\Lambda_B)$ sum to zero. The bounce-averaged trapped particle density, $\hat{N}_i$, is defined in the main text.

Finally, we specialize to tokamak geometry and further assume a background Maxwellian distribution,

$$F(\overline{\mathbf{Y}},\overline{J},\overline{\mu},t)=\frac{N_i(\overline{\mathbf{Y}},t)}{(\pi v_{th}^2)^{3/2}}e^{-H_0/T_i(\overline{\mathbf{Y}})}. \tag{A9}$$

(Note that N_i has no $\overline{\Psi}$ dependence; it is the bounce center density.) To keep the equations analytically tractable, all trapped particles are assumed to be deeply trapped. For a high aspect ratio circular cross section tokamak, the functional forms of the bounce deviations are

$$F_1 = -I\frac{c\sin 2\psi}{2eq}\left(\frac{\partial q}{\partial\beta} - \frac{q}{2\epsilon_a}\frac{\partial\epsilon_a}{\partial\beta}\right) \tag{A10}$$

$$F_2 = -\frac{c}{e}\left(2IR_0\frac{\sqrt{m\epsilon_a\mu B_0}}{q}\right)^{1/2}\sin\psi, \tag{A11}$$

where because of the δ-function integration over $\overline{\Psi}$, the phase angle ψ will be written in terms of s and $\overline{J}$. (Because of notational definitions, F_1 corresponds to the α deviation and F_2 to the radial deviation.) Changing the deviations to bounce-averaged coordinates, substituting, and performing the remaining integrations, we arrive at Eq. (85).

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