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Three-dimensional neoclassical nonlinear kinetic equation for low collisionality axisymmetric tokamak plasmas

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The three-dimensional nonlinear kinetic equation for low collisionality tokamak plasmas with consistent consideration of neoclassical effects is obtained using an approach differing from the standard neoclassical theory technique. This allows treatment of large banana widths and large inverse aspect ratios. The equation is suitable for computer modeling of bootstrap currents and other phenomena arising from non-Maxwellian distributions. The formalism described in this paper, which is for noncanonical variables, might also be of use for the consistent derivation of three-dimensional kinetic equations that treat other effects, for example, additional heating.

I. INTRODUCTION

Research into controlled fusion has now reached thermonuclear relevant parameters. In these plasmas, as in next-step and reactor plasmas, fast ion populations are an important component. For example, minority ion distributions with energies $\lesssim 10$ MeV have been produced with ion cyclotron heating in the Joint European Torus (JET) experiment.[1] It is important to understand the influence of such fast ion populations on plasma behavior. Models of this behavior should allow for both the greatly non-Maxwellian nature of the fast ion distributions (notably of alpha particles in a reactor) and of large deviations of the trajectories of energetic ions from flux surfaces, which have been shown to be important in JET.[2] Previous authors have studied neoclassical effects on fast ion distributions, but although these treatments yielded analytic results, they were not valid for large inverse aspect ratios or large deviations of trajectories from flux surfaces.[3,4] Also, these treatments did not use the full collision operator including self-collisions. In this paper, we describe the derivation of a three-dimensional (3-D) nonlinear kinetic equation that includes these effects and can be used for the numerical study of neoclassical physics associated with such distributions, for example, radial transport and bootstrap currents. The equation is not restricted to energetic particles nor to ions. It might, for example, be used to study bootstrap currents in the presence of non-Maxwellian electron distributions, produced by electron-cyclotron-resonance heating in low-density tokamak plasmas.

Plasma models based on kinetic equations with Coulomb collision terms are widely used in plasma theory.[5,6] The initial kinetic equation is intractable without simplification because it is a complicated integrodifferential equation involving six phase space variables and time. However, in many cases processes with characteristic time scales differing by several orders of magnitude are present, making simplification of the kinetic equation possible. In particular, particles in low collisionality tokamak plasmas undergo comparatively fast motion over gyroangle, poloidal, and toroidal angles. This allows averaging of the equation over "fast" variables and gives 3-D kinetic equations.[7,8] With additional assumptions two-dimensional (2-D) kinetic equations can be obtained.[8–11]

The expression of the kinetic equation in action-angle canonical variables, followed by averaging over the "fast" angular motion, has been used several times since its first use in Ref. 12. In this paper the averaging procedure is applied to the nonlinear kinetic equation for low collisionality tokamak plasmas with noncircular cross section, but for noncanonical variables. These variables are usually more convenient for numerical solution and physical interpretation than canonical variables. The main aim of the paper is to obtain a 3-D kinetic equation suitable for computer modeling with consistent and strict consideration of neoclassical effects allowing for drifts due to magnetic field gradients and curvature and to electric fields. This equation will allow more precise study of bootstrap currents and other phenomena arising from non-Maxwellian distributions.

The approach used in this paper differs from that used in well-known papers devoted to neoclassical theory (for example, Refs. 13–15). The main distinction is that the usual approach is to assume that deviations from Maxwellians are small, solve the kinetic equation for these deviations, and average the result over the flux surfaces. Instead we average the kinetic equation itself, retaining neoclassical effects, and obtain the 3-D equation to be solved. Deviations from Maxwellians are not considered, instead the full nonlinear kinetic problem is treated. In order to retain neoclassical effects during the derivation of the 3-D kinetic equation one needs to keep all terms that lead to the bootstrap current and to neoclassical diffusion. This can be done with a Lagrangian approach using constants of the particle motion.[7–9,12] In this paper the results of Refs. 7 and 8 are generalized and advanced. In particular, we present the formal averaging procedure for the general case of noncanonical variables with consideration of boundary conditions, including those between trapped

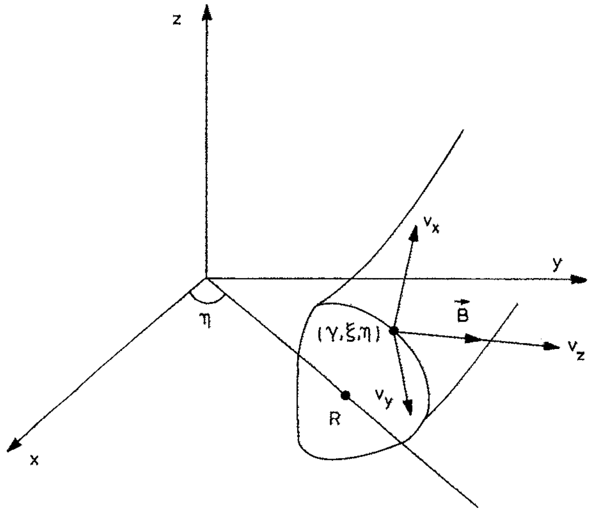

FIG. 1. Cartesian and local coordinate systems.

and passing particles, and obtain formulas suitable for computer simulations. Moreover, averaging is over trajectories with no assumption that they are close to flux surfaces, the usual approximation. This will allow application of the equation to experiments with fast ions (e.g., α particles) whose trajectories do not follow flux surfaces.

The general averaging procedure using noncanonical phase space variables is presented in Secs. II and III, resulting in a 3-D kinetic equation with the Coulomb collision operator averaged over trajectories. This procedure is valid for any three constants of the motion and any three fast variables. In Sec. IV this general procedure is applied to a specific example, neoclassical effects in axisymmetric plasmas for which the drift approximation for particle motion is valid. Formulas for the coefficients in the resulting equation, suitable for computer calculation, are also derived in Sec. IV. The boundary conditions, including those at the trapped passing boundary, are discussed in Sec. V. The procedure for calculating neoclassical toroidal currents and transport fluxes from the solution of this 3-D equation is described in Sec. VI. In Sec. VII we show how the neoclassical ion particle and energy fluxes may be obtained for circular, Maxwellian plasmas: this does not require solution of a kinetic equation, unlike previous derivations,[14,15] which give identical results. Appendices A and B give a number of results convenient for computer treatment of the equation for a suitable choice of variables.

II. COORDINATE SYSTEMS

A toroidal axisymmetric plasma configuration with noncircular cross section (Fig. 1) is considered. In real space (X,Y,Z) toroidal coordinates are used (γ,ξ,η), where γ is any variable that characterizes the magnetic surface, and ξ and η are poloidal and toroidal angles ($\gamma\geqslant 0$, $-\pi<\xi\leqslant\pi, 0\leqslant\eta<2\pi$). A suitable choice for γ might be the "flux surface radius," which is half the width of the surface in the equatorial plane. In velocity space (v_1,v_2,v_3) spherical coordinates (v,θ,φ) are used with the v_3 axis along the magnetic field $\mathbf{B}$ (Fig. 1). Here v is the speed, θ is the pitch angle, and φ is the gyroangle ($v\geqslant 0, 0\leqslant\theta\leqslant\pi, 0\leqslant\varphi<2\pi$). The system $(\gamma,\xi,\eta,v,\theta,\varphi)$ is called the local coordinate system, which, for convenient presentation of the kinetic equation, is denoted as x:

$$x^1\equiv\gamma,\quad x^2\equiv\xi,\quad x^3\equiv\eta,\quad x^4\equiv v,\quad x^5\equiv\theta,\quad x^6\equiv\varphi,$$

$$x\equiv(x^1,x^2,x^3,x^4,x^5,x^6).$$

Before averaging one needs to transform into a coordinate system of constants of motion and "fast" variables. In general, suitable coordinate systems arise from the ordinary differential equations which describe particle motion in collisionless plasmas. Constants of the motion can be, for example, values of variables at a given point on the particle trajectory. These values fix the trajectory and after averaging we obtain an equation that describes the evolution of trajectories as a whole through changes to constants of motion due to collisions. We stress that the results of Sec. III are valid for any three independent constants of the motion and three fast variables.

In Sec. IV, for the consideration of neoclassical effects in axisymmetric tokamaks, we shall use the drift approximation for particle motion to derive the coefficients of the three-dimensional (3-D) equation. It is well known that three constants of drift motion in axisymmetric collisionless toroidal plasmas exist.[16] These constants will be denoted as γ_0, v_0, and θ_0 and should be chosen to give the most convenient equation for a numerical solution. A suitable choice is, respectively, the flux surface radius at the inside of the drift surface (or at the bounce point for trapped particles), a generalized particle speed derived from the sum of kinetic and potential energies, and the pitch angle, where the particle crosses the equatorial plane at the outermost point of its trajectory, which can be on the coleg or counterleg for trapped particles, ($\gamma_{0,\min}\leqslant\gamma_0\leqslant\gamma_{0,\max}, v_{0,\min}\leqslant v_0<\infty, 0\leqslant\theta_0\leqslant\pi$). Details of the transformation between local variables and this choice for γ_0, v_0, and θ_0 are given in Appendix A. The following notation for the "constants of motion" coordinate system $\bar{x}$ will be used in Secs. III and IV:

$$\bar{x}^1\equiv\gamma_0,\quad \bar{x}^2\equiv\xi,\quad \bar{x}^3\equiv\eta,\quad \bar{x}^4\equiv v_0,\quad \bar{x}^5\equiv\theta_0,\quad \bar{x}^6\equiv\varphi,$$

$$\bar{x}\equiv(\bar{x}^1,\bar{x}^2,\bar{x}^3,\bar{x}^4,\bar{x}^5,\bar{x}^6).$$

III. AVERAGED 3-D KINETIC EQUATION

We start from the most general kinetic equation with the Landau collision operator,[5,6]

$$\frac{df_\alpha}{dt}=\sum_\beta \nabla\cdot\mathbf{j}_\beta(f_\alpha,f_\beta), \tag{1}$$

with f_α and f_β the distribution functions of particle species α and β. The left-hand side describes changes in the distribution function due to motion of particles in a collisionless plasma under the influence of external forces. The right-hand side describes changes due to Coulomb collisions, with the summation over β over all particle species. Strictly speaking, we have a set of equations, one for each species α. The form in which Eq. (1) is written is independent of the coordinate system. In Cartesian coordinates and SI units the flux $\mathbf{j}_\beta$ has the following components:

$$\mathbf{j}_\beta=(0,0,0,j_\beta^{v_x},j_\beta^{v_y},j_\beta^{v_z}),$$

where

$$j_\beta^{v_i}=\frac{(e_\alpha e_\beta)^2\ln\Lambda_{\alpha\beta}}{\epsilon_0^2 m_\alpha}\left(\frac{1}{m_\beta}\frac{\partial\varphi_\beta}{\partial v_i}f_\alpha-\frac{1}{m_\alpha}\frac{\partial^2\psi_\beta}{\partial v_i\,\partial v_k}\frac{\partial f_\alpha}{\partial v_k}\right),$$

with i, $k=x,y,z$; $\ln\Lambda_{\alpha\beta}$ is the Coulomb logarithm; and e_α, e_β, and m_α, m_β are the particle charges and masses. Summation over repeated indices is assumed (except for α and β). The components $j_\beta^{v_i}$ may be expressed in terms of Rosenbluth potentials,[17,5]

$$\frac{\partial\varphi_\beta}{\partial v_i}=-\frac{1}{8\pi}\int U_{ik}\frac{\partial f_\beta(t,x,y,z,v_1',v_2',v_3')}{\partial v_k'}\,dv_1'\,dv_2'\,dv_3', \tag{2}$$

$$\frac{\partial^2\psi_\beta}{\partial v_i\partial v_k}=-\frac{1}{8\pi}\int U_{ik}f_\beta(t,x,y,z,v_1',v_2',v_3')\,dv_1'\,dv_2'\,dv_3', \tag{3}$$

$$U_{ik}=\frac{\partial^2 u}{\partial v_i\partial v_k}=\frac{\delta_{ik}}{u}-\frac{u_iu_k}{u^3},$$

with $\mathbf{u}=\mathbf{v}-\mathbf{v}'$ the relative speed, $u=|\mathbf{u}|$, and δ_{ik} the Kronecker symbol.

The left-hand side in Eq. (1) is transformed using

$$\nabla\cdot\frac{d\mathbf{r}_6}{dt}=0,$$

for Hamiltonian systems, where

$$\frac{d\mathbf{r}_6}{dt}=\left(\frac{d\bar{x}^1}{dt},\ldots,\frac{d\bar{x}^6}{dt}\right),$$

and making use of

$$\frac{d\gamma_0}{dt}=0,\quad\frac{dv_0}{dt}=0,\quad\frac{d\theta_0}{dt}=0.$$

(Note that in this section γ_0, v_0, and θ_0 are any three independent constants of the motion.) Thus the left-hand side of Eq. (1) takes the form

$$\frac{df_\alpha}{dt}=\frac{\partial f_\alpha}{\partial t}+\sum_{n=2,3,6}\frac{1}{\sqrt{g}}\frac{\partial}{\partial\bar{x}^n}\left(\sqrt{g}\frac{d\bar{x}^n}{dt}f_\alpha\right).$$

The right-hand side in Eq. (1) in the new coordinates $\bar{x}$ transforms to

$$\sum_\beta\nabla\cdot\mathbf{j}_\beta(f_\alpha,f_\beta)=\sum_\beta\sum_{n=1,\ldots,6}\frac{1}{\sqrt{g}}\frac{\partial}{\partial\bar{x}^n}\left(\sqrt{g}\frac{\partial\bar{x}^n}{\partial v_i}j_\beta^{v_i}\right),$$

where $\sqrt{g}$ is the Jacobian of the transformation from Cartesian coordinates to $\bar{x}$ and the expression relating the contravariant components of $\mathbf{j}_\beta$ in different coordinate systems,

$$j_\beta^{\bar{x}^n}=\frac{\partial\bar{x}^n}{\partial v_i}j_\beta^{v_i}$$

has been used. For convenience we introduce a normalizing Coulomb relaxation time τ_c, but emphasize that spatial variations of density, temperature, etc., are treated in the formalism:

$$\tau_c=\left(\frac{m_\alpha}{2}\right)^{1/2}\frac{16\pi\epsilon_0^2E_c^{3/2}}{n_cZ_\alpha^2e^4\ln\Lambda}.$$

We also introduce the functions of f_β,

$$a_\beta^{ik}(f_\beta)=-\frac{4\pi Z_\beta^2\ln\Lambda_{\alpha\beta}}{n_c\ln\Lambda}\frac{\partial^2\psi_\beta}{\partial v_i\,\partial v_k},$$

$$b_\beta^i(f_\beta)=\frac{4\pi Z_\beta^2\ln\Lambda_{\alpha\beta}}{n_c\ln\Lambda}\frac{m_\alpha}{m_\beta}\frac{\partial\varphi_\beta}{\partial v_i}.$$

Here e is the electron charge, $Z_\alpha=e_\alpha/|e|$, n_c is a characteristic density, E_c is a characteristic energy (temperature), and $\ln\Lambda$ is a characteristic Coulomb logarithm. Using this notation, the right-hand side in Eq. (1) can be expressed as

$$\frac{v_c^3}{\tau_c}\frac{1}{\sqrt{g}}\frac{\partial}{\partial\bar{x}^n}\left[\sqrt{g}\frac{\partial\bar{x}^n}{\partial v_i}\left(\frac{\partial f_\alpha}{\partial v_k}\sum_\beta a_\beta^{ik}(f_\beta)+f_\alpha\sum_\beta b_\beta^i(f_\beta)\right)\right],$$

with $v_c^2=2E_c/m_\alpha$. Thus in the new coordinates $\bar{x}$, Eq. (1) can be rewritten as

$$\frac{\partial f_\alpha}{\partial t}+\sum_{n=2,3,6}\frac{1}{\sqrt{g}}\frac{\partial}{\partial\bar{x}^n}\left(\sqrt{g}\frac{d\bar{x}^n}{dt}f_\alpha\right)$$
$$=\frac{v_c^3}{\tau_c}\sum_{n=1,\ldots,6}\frac{1}{\sqrt{g}}\frac{\partial}{\partial\bar{x}^n}\left[\sqrt{g}\frac{\partial\bar{x}^n}{\partial v_i}\left(\frac{\partial f_\alpha}{\partial v_k}\sum_\beta a_\beta^{ik}(f_\beta)\right.\right.$$
$$\left.\left.+f_\alpha\sum_\beta b_\beta^i(f_\beta)\right)\right], \tag{4}$$

with i, $k=1,2,3$.

We now make the assumption of low collisionality, which is that the characteristic times for motion over "fast" variables $\bar{x}^2$, $\bar{x}^3$, and $\bar{x}^6$ (in Sec. IV these will be poloidal, toroidal, and gyroangles) are much less than τ_c. If the largest of these characteristic times is τ, then τ/τ_c is a small parameter and, defining $\hat{t}=t/\tau_c$ and $\hat{\hat{t}}=t/\tau$, we search for the solution of Eq. (4) in the form

$$f_\alpha(t,\bar{x})=f_\alpha^0(t,\bar{X})+\frac{\tau}{\tau_c}f_\alpha^{(1)}(t,\bar{X},\tilde{X})+\left(\frac{\tau}{\tau_c}\right)^2f_\alpha^{(2)}(t,\bar{X},\tilde{X})$$
$$+\ldots, \tag{5}$$

where $\bar{X}=(\gamma_0,v_0,\theta_0)$ are constants of motion and $\tilde{X}=(\xi,\eta,\varphi)$ are fast variables [with $d(\ln\tilde{X})/d\hat{\hat{t}}\sim d(\ln f)/d\hat{t}$]. The aim of the averaging procedure is to find an equation for $f_\alpha^0(t,\bar{X})$. One approach would be to integrate Eq. (4) over the fast variables $\tilde{X}$, retaining terms of the desired order. Instead we use a more general approach, seeking an equation for $f_\alpha^0(t,\bar{X})$ with the following structure:

$$A^0(\bar{X};f_\alpha^0)+\frac{\tau}{\tau_c}A^{(1)}(\bar{X};f_\alpha^0)+\left(\frac{\tau}{\tau_c}\right)^2A^{(2)}(\bar{X};f_\alpha^0)+\cdots=0, \tag{6}$$

and choose $f_\alpha^{(i)}$ and $A^{(i)}(i=0,1,2,\ldots)$ to satisfy Eq. (4). These terms $A^{(i)}$ will be found by splitting Eq. (4) into two components, with one of the components independent of $\tilde{X}$. This procedure gives identical results to direct integration over the fast variables $\tilde{X}$ if all the terms in Eq. (4) are integrable functions. However, if the terms are not integrable, then the direct integration method cannot formally be used, but the approach used here is still valid. [For example, the radial diffusion term arising in neoclassical transport is not integrable in the trapped particle region. This is because a term of the form $\partial/\partial\gamma_0(D\partial f/\partial\gamma_0)$, with $D \sim 1/|\cos\theta|$, is to be averaged and $\partial/\partial\gamma_0(1/|\cos\theta|)$ is not integrable since the integration is to the reflection points and $\partial/\partial\gamma_0(1/|\cos\theta|)\sim 1/\cos^2\theta$. The direct integration method requires that $\partial D/\partial\gamma_0$ is integrable, whereas the method used here requires only that D is integrable.]

Solutions f_α^0 to Eq. (6) to zeroth-, first-,..., order accuracy in τ/τ_c may then be obtained by solving $A^0(\bar{X};f_\alpha^0)=0, A^0(\bar{X};f_\alpha^0)+(\tau/\tau_c)A^{(1)}(\bar{X};f_\alpha^0)=0$, etc. Multiplication of Eq. (4) by $\tau_c\sqrt{g}$ followed by substitution of Eqs. (5) and (6) gives

$$
\begin{aligned}
&A^0(\bar{X};f_\alpha^0)+\frac{\tau}{\tau_c}A^{(1)}(\bar{X};f_\alpha^0)+\left(\frac{\tau}{\tau_c}\right)^2 A^{(2)}(\bar{X};f_\alpha^0)+\cdots\\
&\quad+\sqrt{g}\frac{\partial}{\partial\hat{t}}\left[f_\alpha^0+\frac{\tau}{\tau_c}f_\alpha^{(1)}+\left(\frac{\tau}{\tau_c}\right)^2 f_\alpha^{(2)}+\cdots\right]+\frac{\tau_c}{\tau}\\
&\quad\times\sum_{n=2,3,6}\frac{\partial}{\partial\bar{x}^n}\left\{\sqrt{g}\frac{d\bar{x}^n}{d\hat{t}}\left[\frac{\tau}{\tau_c}f_\alpha^{(1)}+\left(\frac{\tau}{\tau_c}\right)^2 f_\alpha^{(2)}+\cdots\right]\right\}\\
&\quad=v_c^3\sum_{n=1,\dots,6}\frac{\partial}{\partial\bar{x}^n}\left\{\sqrt{g}\frac{\partial\bar{x}^n}{\partial v_i}\left[\frac{\partial}{\partial v_k}\left(f_\alpha^0+\frac{\tau}{\tau_c}f_\alpha^{(1)}+\cdots\right)\right.\right.\\
&\quad\times\sum_\beta a_\beta^{ik}\left(f_\beta^0+\frac{\tau}{\tau_c}f_\beta^{(1)}+\cdots\right)+\left(f_\alpha^0+\frac{\tau}{\tau_c}f_\alpha^{(1)}\right.\\
&\quad\left.\left.\left.+\cdots\right)\times\sum_\beta b_\beta^i\left(f_\beta^0+\frac{\tau}{\tau_c}f_\beta^{(1)}+\cdots\right)\right]\right\}. \qquad (7)
\end{aligned}
$$

The last term on the left-hand side of the equation was simplified using

$$
\begin{aligned}
&\sum_{n=2,3,6}\frac{1}{\sqrt{g}}\frac{\partial}{\partial\bar{x}^n}\left(\sqrt{g}\frac{d\bar{x}^n}{dt}f_\alpha^0\right)\\
&\quad=f_\alpha^0\left[\nabla\cdot\frac{d\mathbf{r}_6}{dt}-\sum_{n=1,4,5}\frac{1}{\sqrt{g}}\frac{\partial}{\partial\bar{x}^n}\left(\sqrt{g}\frac{d\bar{x}^n}{dt}\right)\right]=0,
\end{aligned}
$$

which follows since f_α^0 is independent of $\bar{x}^n$ for $n=2,3,6, \nabla\cdot(d\mathbf{r}_6/dt)=0$ and $d\bar{x}^n/dt=0$ for $n=1,4,5$ (constants of motion).

In the zeroth order [remembering that $a_\beta^{ik}(f)$ and $b_\beta^{ik}(f)$ are linear functions of f], the following expression immediately follows from Eq. (7):

$$
\begin{aligned}
&A^0(\bar{X};f_\alpha^0)+\sqrt{g}\frac{\partial f_\alpha^0}{\partial\hat{t}}+\sum_{n=2,3,6}\frac{\partial}{\partial\bar{x}^n}\left(\sqrt{g}\frac{d\bar{x}^n}{d\hat{t}}f_\alpha^{(1)}\right)\\
&\quad=v_c^3\sum_{n=1,\dots,6}\frac{\partial}{\partial\bar{x}^n}\left[\sqrt{g}\frac{\partial\bar{x}^n}{\partial v_i}\left(\frac{\partial f_\alpha^0}{\partial v_k}\sum_\beta a_\beta^{ik}(f_\beta^0)\right.\right.\\
&\quad\left.\left.+f_\alpha^0\sum_\beta b_\beta^i(f_\beta^0)\right)\right]. \qquad (8)
\end{aligned}
$$

In Eq. (8) there are two unknown terms, A^0 and $f_\alpha^{(1)}$: it is convenient to define these using the following procedure. Terms in Eq. (8) are split into two components: the first independent of $\tilde{X}$ and the second depending on both $\bar{X}$ and $\tilde{X}$. The resulting two components of Eq. (8) are each set to zero and give A^0 and $f_\alpha^{(1)}$, respectively. Formally, there is no unique choice for these components: we use the definition that ensures both that f_α^0 is the distribution function in the space of constants of motion $\bar{X}$, and that the resulting equation for f_α^0 is in the form of the divergence of a flux in this space $\bar{X}$. The choice of splitting procedure is such that the coefficients in the flux will be the appropriate diffusion and convection coefficients averaged over the three fast variables $\tilde{X}$, thus giving the flux a clear physical interpretation.

We define the component of any integrable function $a(\bar{x})$ that is independent of $\tilde{X}$ as

$$
\langle a\rangle\equiv\langle a\rangle_{\xi,\eta,\varphi}\equiv\frac{1}{H}\int_{\Delta\xi}d\xi\int_{\Delta\eta}d\eta\int_{\Delta\varphi}d\varphi\, a(\bar{x})\sqrt{g},
$$

where integrals are taken over the ranges of ξ, η, and φ explored by particles described by the set of constants of motion $\bar{X}$, and H is independent of $\tilde{X}$ and has the dimensions of $d\xi\, d\eta\, d\varphi$. The actual value of H is unimportant, as it will not appear in the final equation for f_α^0. We emphasize that the limits of integration can, in general, depend on $\bar{X}$. Moreover the way in which the integral is taken can differ for different coordinates $\tilde{X}$ (see, for example, the case described in Sec. IV). If the $\langle a\rangle$ component is known then the remaining component $\{a\}$ of $a(\bar{x})$ can be defined as

$$
\{a\}=a\sqrt{g}-\langle a\rangle.
$$

Equating to zero the component of Eq. (8) that is independent of $\tilde{X}$ gives

$$
\begin{aligned}
A^0(\bar{X};f_\alpha^0)=&-\langle 1\rangle\frac{\partial f_\alpha^0}{\partial\hat{t}}+v_c^3\sum_{n=1,4,5}\frac{\partial}{\partial\bar{x}^n}\left(\frac{\partial f_\alpha^0}{\partial\bar{x}^m}\left\langle\frac{\partial\bar{x}^n}{\partial v_i}\frac{\partial\bar{x}^m}{\partial v_k}\right.\right.\\
&\left.\left.\times\sum_\beta a_\beta^{ik}(f_\beta^0)\right\rangle+f_\alpha^0\left\langle\frac{\partial\bar{x}^n}{\partial v_i}\sum_\beta b_\beta^i(f_\beta^0)\right\rangle\right). \qquad (9)
\end{aligned}
$$

The $n=2,3,6$ terms in the summation in Eq. (8) appear in the other equation, that for $f_\alpha^{(1)}$. In deriving Eq. (9) the following relation, valid since f_α^0 is independent of $\tilde{X}$, was used:

$$
\frac{\partial f_\alpha^0}{\partial v_k}=\sum_{m=1,4,5}\frac{\partial f_\alpha^0}{\partial\bar{x}^m}\frac{\partial\bar{x}^m}{\partial v_k}.
$$

The remaining component of Eq. (8), that depending on both $\bar{X}$ and X, determines $f_\alpha^{(1)}$ and is

$$\sum_{n=2,3,6} \frac{\partial}{\partial \bar{x}^n}\left(\sqrt{\bar{g}}\frac{d\bar{x}^n}{d\hat{t}} f_\alpha^{(1)}\right)$$

$$= -\{1\}\frac{\partial f_\alpha^0}{\partial \hat{t}} + v_c^3 \sum_{n=1,4,5} \frac{\partial}{\partial \bar{x}^n}\left[\frac{\partial f_\alpha^0}{\partial \bar{x}^m}\left(\frac{\partial \bar{x}^n}{\partial v_i}\frac{\partial \bar{x}^m}{\partial v_k}\right.\right.$$

$$\left.\left.\times \sum_\beta a_\beta^{ik}(f_\beta^0)\right) + f_\alpha^0\left(\frac{\partial \bar{x}^n}{\partial v_i}\sum_\beta b_\beta^i(f_\beta^0)\right)\right]$$

$$+ v_c^3 \sum_{n=2,3,6} \frac{\partial}{\partial \bar{x}^n}\left(\frac{\partial f_\alpha^0}{\partial \bar{x}^m}\frac{\partial \bar{x}^n}{\partial v_i}\frac{\partial \bar{x}^m}{\partial v_k}\sum_\beta a_\beta^{ik}(f_\beta^0)\sqrt{\bar{g}}\right.$$

$$\left. + f_\alpha^0 \frac{\partial \bar{x}^n}{\partial v_i}\sum_\beta b_\beta^i(f_\beta^0)\sqrt{\bar{g}}\right). \tag{10}$$

If we have a solution of Eq. (10), $f_\alpha^{(1)}$, then this solution plus any function of $\bar{X}$ will also satisfy Eq. (10). It is most convenient to choose the solution satisfying $\langle f_\alpha^{(1)}\rangle = 0$, which gives the simplest expression for $A^{(1)}$. Moreover, all $f_\alpha^{(i)}$ for $i=1,2,\ldots$, can be chosen to satisfy $\langle f_\alpha^{(i)}\rangle = 0$ and thus $\langle f_\alpha\rangle = f_\alpha^0\langle 1\rangle$ is independent of $f_\alpha^{(i)}$. Using Eq. (9) in Eq. (6), and neglecting higher-order terms, gives one of the main results of this paper: the averaged, nonlinear 3-D kinetic equation for low collisionality plasmas,

$$\frac{\partial f_\alpha^0}{\partial t} = \frac{v_c^3}{\tau_c}\sum_{n=1,4,5}\frac{1}{\langle 1\rangle}\frac{\partial}{\partial \bar{x}^n}\left(\frac{\partial f_\alpha^0}{\partial \bar{x}^m}\left\langle\frac{\partial \bar{x}^n}{\partial v_i}\frac{\partial \bar{x}^m}{\partial v_k}\sum_\beta a_\beta^{ik}(f_\beta^0)\right\rangle\right.$$

$$\left. + f_\alpha^0\left\langle\frac{\partial \bar{x}^n}{\partial v_i}\sum_\beta b_\beta^i(f_\beta^0)\right\rangle\right), \tag{11}$$

where $f_\alpha^0 \equiv f_\alpha^0(t,\bar{X}) \equiv f_\alpha^0(t,\gamma_0,v_0,\theta_0)$.

In principle this equation, with the appropriate boundary conditions and particle and energy sources, can be solved to produce all the fluxes (including currents) arising from neoclassical effects. It would yield a self-consistent distribution function, which, if differing significantly from Maxwellian, would give different fluxes from those derived previously for Maxwellian distributions.

Equation (11) allows determination of f_α^0, but with an error $O(\tau/\tau_c)$. To this order,

$$f_\alpha = f_\alpha^0 + O(\tau/\tau_c),$$

but to find f_α^0 (and later f_α) with greater accuracy the term $A^{(1)}(\bar{X};f_\alpha^0)$ in Eq. (6) must be determined. This can be done in the same manner as for $A^0(\bar{X};f_\alpha^0)$, but for consideration of the terms $O(\tau/\tau_c)$ in Eq. (7). This gives

$$f_\alpha = f_\alpha^0 + \frac{\tau}{\tau_c} f_\alpha^{(1)} + O\left[\left(\frac{\tau}{\tau_c}\right)^2\right],$$

where f_α^0 is the solution of

$$A^0(\bar{X};f_\alpha^0) + \frac{\tau}{\tau_c}A^{(1)}(\bar{X};f_\alpha^0) = 0$$

and $f_\alpha^{(1)}$ is the solution of Eq. (10) with f_α^0 the solution of Eq. (11).

IV. COEFFICIENTS OF THE 3-D EQUATION FOR DRIFT MOTION IN AXISYMMETRIC PLASMAS

Section III was devoted to a general method for the derivation of 3-D kinetic equations. In this section this method is applied to neoclassical processes in axisymmetric plasmas. The coefficients of the resulting equation, Eq. (11), are put in a form suitable for computer calculation, with the help of additional assumptions appropriate to a neoclassical description of tokamak transport. These are that the plasma is axisymmetric and that the drift approximation for particle motion is valid. This second assumption means that finite-Larmor radius effects are neglected (unlike in gyrokinetic treatments): however, we emphasize that the banana width and inverse aspect ratio need not be small.

The first coefficient appearing in Eq. (11), A_{nm}, is given by

$$A_{nm} \equiv \left\langle\frac{\partial \bar{x}^n}{\partial v_i}\frac{\partial \bar{x}^m}{\partial v_k}\sum_\beta a_\beta^{ik}(f_\beta^0)\right\rangle$$

$$= \sum_\beta \frac{4\pi Z_\beta^2 \ln \Lambda_{\alpha\beta}}{n_c \ln \Lambda}\frac{1}{8\pi}\left\langle\frac{\partial \bar{x}^n}{\partial v_i}\frac{\partial \bar{x}^m}{\partial v_k}\int U_{ik} f_\beta^0(t,x,y,z,v_1',v_2',v_3')\,dv_1'\,dv_2'\,dv_3'\right\rangle$$

$$= \sum_\beta \frac{Z_\beta^2 \ln \Lambda_{\alpha\beta}}{2n_c \ln \Lambda}\left\langle\frac{\partial \bar{x}^n}{\partial x^l}\frac{\partial \bar{x}^m}{\partial x^j}\frac{\partial x^l}{\partial v_i}\frac{\partial x^j}{\partial v_k}\int_0^\infty\int_0^\pi\int_0^{2\pi} U_{ik} f_\beta^0[t,\bar{X}(x')]\,v'^2\sin\theta'\,dv'\,d\theta'\,d\varphi'\right\rangle, \tag{12}$$

with $x' \equiv (\gamma,\xi,\eta,v',\theta',\varphi')$; $n,m=1,4,5$; $l,j=4,5,6$ (since $\partial x^l/\partial v_i = 0$ for $l=1,2,3$, $i=1,2,3$). In the drift approximation, γ_0,v_0,θ_0 are independent of the gyroangle φ, that is, $\bar{X}' \equiv \bar{X}(\gamma,\xi,\eta,v',\theta')$ (see Appendix A). Thus the derivatives $\partial \bar{x}^n/\partial x^l$ and $f_\beta^0(t,\bar{X}')$ are independent of φ and φ' giving

$$A_{nm} = \sum_\beta \frac{Z_\beta^2 \ln \Lambda_{\alpha\beta}}{2n_c \ln \Lambda}\left\langle\frac{\partial \bar{x}^n}{\partial x^l}\frac{\partial \bar{x}^m}{\partial x^j}\int_0^\infty\int_0^\pi \bar{U}_{lj} f_\beta^0(t,\bar{X}')\,v'^2\right.$$

$$\left.\times\sin\theta'\,dv'\,d\theta'\right\rangle_{\xi,\eta}, \tag{13}$$

where

$$\bar{U}_{lj} \equiv \int_0^{2\pi} \int_0^{2\pi} \frac{\partial x^l}{\partial v_i} \frac{\partial x^j}{\partial v_k} U_{ik}\, d\varphi\, d\varphi'.$$

Moreover, $\partial \bar{x}^n / \partial x^6 = 0$ for $n = 1,...,5$ (since $x^6 = \varphi$), and thus $l,j = 4,5$ in Eq. (13).

In the same way, the second coefficient in Eq. (11), B_n, may be obtained,

$$B_n \equiv \left\langle \frac{\partial \bar{x}^n}{\partial v_i} \sum_\beta b^i_\beta (f^0_\beta) \right\rangle$$

$$= -\sum_\beta \frac{Z^2_\beta \ln \Lambda_{\alpha\beta}}{2n_c \ln \Lambda} \frac{m_\alpha}{m_\beta}$$

$$\times \left\langle \frac{\partial \bar{x}^n}{\partial x^l} \int_0^\infty \int_0^\pi \bar{U}'_{lj} \frac{\partial f^0_\beta (t, \bar{X}')}{\partial x'^j} v'^2 \sin\theta'\, dv'\, d\theta' \right\rangle_{\xi,\eta}, \quad (14)$$

where

$$\bar{U}'_{lj} \equiv \int_0^{2\pi} \int_0^{2\pi} \frac{\partial x^l}{\partial v_i} \frac{\partial x'^j}{\partial v'_k} U_{ik}\, d\varphi\, d\varphi'.$$

Analytic formulas for the matrix elements $\bar{U}_{lj}$ and $\bar{U}'_{lj}$ are given in Appendix B.

Finally, Eq. (11) can be written as

$$\frac{\partial f^0_\alpha}{\partial t} = \frac{v^3_c}{\tau_c} \sum_{n=1,4,5} \frac{1}{\langle 1 \rangle} \frac{\partial}{\partial \bar{x}^n} \left[\sum_{m=1,4,5} \left(A_{nm} \frac{\partial f^0_\alpha}{\partial \bar{x}^m} \right) + B_n f^0_\alpha \right]. \quad (15)$$

The coefficients A_{nm} and B_n describe radial diffusion (A_{11}), pitch angle scattering (A_{55}), collisional slowing down (B_4), etc., and are given by Eqs. (13) and (14), with $\langle 1 \rangle$ given by

$$\langle 1 \rangle = 2\pi \int_{\Delta\xi} d\xi \int_{\Delta\eta} d\eta \sqrt{g}.$$

Although analytic formulas for $\bar{U}_{lj}$ and $\bar{U}'_{lj}$ exist (Appendix B), calculation of the coefficients in Eq. (15) still requires considerable computer time. However, the assumption of axisymmetry allows further simplification of the coefficients through analytic integration over toroidal angle η.

We make the distinction between two groups of particles in axisymmetric magnetic configurations: passing and trapped particles. Passing particles move in the same direction [$\sigma \equiv \mathrm{sgn}(\cos\theta) = 1$] or in the opposite direction ($\sigma = -1$) to the magnetic field. Trapped particles "bounce" in the nonuniform magnetic field and thus have $\sigma = \pm 1$. Averaged quantities are calculated for the two groups of particles in different ways. For passing particles,

$$\langle a \rangle^\sigma_{\xi,\eta} \equiv \int_{\xi^\sigma_{\min}(\bar{X})}^{\xi^\sigma_{\max}(\bar{X})} \int_{\eta^\sigma_{\min}(\bar{X})}^{\eta^\sigma_{\max}(\bar{X})} (a\sqrt{g})_\sigma\, d\xi\, d\eta, \quad (16)$$

whereas for trapped particles,

$$\langle a \rangle^{\mathrm{tr}}_{\xi,\eta} \equiv \sum_{\sigma=-1,1} \int_{\xi^\sigma_{\min}(\bar{X})}^{\xi^\sigma_{\max}(\bar{X})} \int_{\eta^\sigma_{\min}(\bar{X})}^{\eta^\sigma_{\max}(\bar{X})} (a\sqrt{g})_\sigma\, d\xi\, d\eta. \quad (17)$$

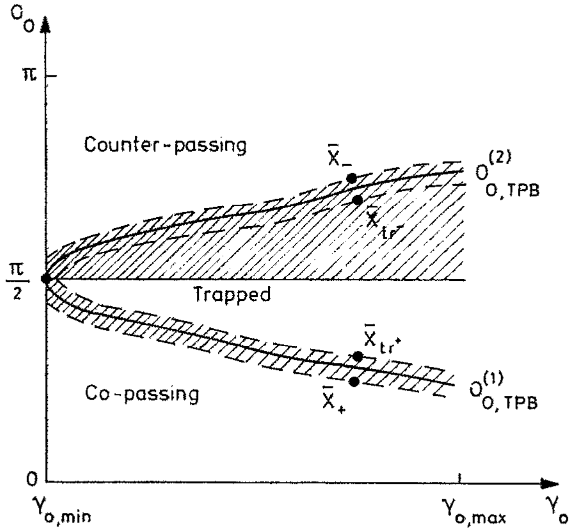

FIG. 2. Trapped and passing particle regions in (γ_0, θ_0) space. In the dashed area the equation for the averaged distribution function $f^0_\alpha(t,\bar{X})$ need not be solved for.

In Eqs. (16) and (17), $\xi^\sigma_{\min}(\bar{X})$, $\xi^\sigma_{\max}(\bar{X})$, $\eta^\sigma_{\min}(\bar{X})$, and $\eta^\sigma_{\max}(\bar{X})$ denote the limits of phase space permitted for particles with coordinates $\bar{X}$, and σ denotes that functions within integrals should be considered as functions of constants of the motion $\bar{x}$ with the appropriate sign of σ. The summation in Eq. (17) is required since the motions of a trapped particle co and counter to the magnetic field should not be treated separately, rather the trajectory should be considered as a whole. For axisymmetric plasmas, since all initial values of η are permitted for any $\bar{X}$, $\eta^\sigma_{\min}(\bar{X}) = 0$ and $\eta^\sigma_{\max}(\bar{X}) = 2\pi$. Also, for up–down symmetric, axisymmetric plasmas, $\xi^-_{\min}(\bar{X}) = \xi^+_{\min}(\bar{X}) = -\xi^-_{\max}(\bar{X}) = -\xi^+_{\max}(\bar{X})$.

In the case of axisymmetry, therefore, averaging over toroidal angle η simplifies Eqs. (16) and (17),

$$\langle a \rangle^\pm_{\xi,\eta} = 2\pi \int_{-\pi}^{\pi} (a\sqrt{g})_{\sigma=\pm 1}\, d\xi, \quad (18)$$

$$\langle a \rangle^{\mathrm{tr}}_{\xi,\eta} = 2\pi \sum_{\sigma=-1,1} \int_{\xi_{\min}(\bar{X})}^{\xi_{\max}(\bar{X})} (a\sqrt{g})_\sigma\, d\xi. \quad (19)$$

Here $\xi_{\min}$ and $\xi_{\max}$ are poloidal angles at the reflection points, with, for up–down symmetry, $\xi_{\min} = -\xi_{\max}$. [These angles may be derived by putting $\theta^i = \pi/2$ in Eqs. (A1)–(A3) in Appendix A.]

It is important to appreciate that, because of the averaging procedure described, the whole trapped particle trajectory is considered as one object. For trapped particles, there are two pitch angles where the trajectory crosses the equatorial plane: one for the coleg and one for the counterleg, with one satisfying $\theta^{(1)}_{0,\mathrm{TPB}} < \theta_0 \leqslant \pi/2$, and the other, $\pi/2 < \theta_0 < \theta^{(2)}_{0,\mathrm{TPB}}$. Here $\theta^{(1)}_{0,\mathrm{TPB}}$ and $\theta^{(2)}_{0,\mathrm{TPB}}$ are functions of γ_0 and v_0 and are the values of θ_0 at the trapped–passing boundary (see Fig. 2). Thus, one object is described by two values of θ_0. But because the values of averaged quantities at these points are equal as they correspond to one and the same object, one need only solve for f_α^0 for θ_0 in the range $\theta_{0,\mathrm{TPB}}^{(1)} < \theta_0 < \pi/2$.

Computer calculation of each A_{nm} and B_n involves numerical integration over ξ, v', and θ'. These coefficients are required for every combination of γ_0, v_0, and θ_0, resulting in a very large number $O(N^6)$ arithmetic operations for each time t, where N is the number of points of each variable. The number of operations can be reduced to $O(N^5)$ for each t if one can find an appropriate series expansion for $f_\beta^0(\bar{X}')$ in, for example, the θ' coordinate. If this is possible, the θ' integral can be calculated once at the beginning of the program and used later for each t. This will be an efficient algorithm if the number of terms in the series can be taken small in comparison with N.

V. TRAPPED–PASSING BOUNDARY, BOUNDARY, AND INITIAL CONDITIONS

The averaging method is not valid for particles so near the trapped–passing boundary (TPB) that $\tau \sim \tau_c$. Thus, the phase space is cut by a narrow transition layer around the TPB for which special treatment is required (Fig. 2). This treatment is discussed in this section.

In the averaging procedure the trajectory of a trapped particle has been considered as a whole, and one need find $f_\alpha^0(t,\bar{X})$ only for $\theta_{0,\mathrm{TPB}}^{(1)} < \theta_0 < \pi/2$. This means that we need to describe particles entering or leaving the trapped–passing region only through one boundary, $\theta_0 = \theta_{0,\mathrm{TPB}}^{(1)}$ (see Fig. 2).

We proceed from the assumption that, due to Coulomb collisions and the absence of sources at the TPB layer, the unaveraged distribution function f_α, and the normal component of the unaveraged flux $\mathbf{j} = \Sigma_\beta j_\beta$, are continuous functions of $\bar{x}$ coordinates. Then for f_α^0, with $O(\tau/\tau_c)$ accuracy, it is straightforward to derive the following conditions at the TPB:

$$f_\alpha^0(t,\bar{X}_+) = f_\alpha^0(t,\bar{X}_-) = f_\alpha^0(t,\bar{X}_{\mathrm{tr}+}), \tag{20}$$

where "+," "−," and "tr$^+$" denote that boundary points on the transition layer are taken from the copassing, counterpassing, and trapped regions, respectively (Fig. 2).

Averaging the equations for continuity of the component of the flux normal to the TPB, $\mathbf{j}\cdot\mathbf{n}_{\mathrm{TPB}}$, where $\mathbf{n}_{\mathrm{TPB}} = \nabla F/|\nabla F|$ is the unit vector perpendicular to the TPB surface, and $F(\bar{X}) = 0$ defines the TPB surface, one can obtain with the same order of accuracy as Eq. (20),

$$\sum_{n=1,4,5} \frac{\langle f^{\bar{x}^n}(t,\bar{X}_+,\tilde{X})\rangle^+}{|\nabla F(\bar{X}_+)|}\frac{\partial F(\bar{X}_+)}{\partial \bar{x}^n} + \frac{\langle f^{\bar{x}^n}(t,\bar{X}_-,\tilde{X})\rangle^-}{|\nabla F(\bar{X}_-)|}\frac{\partial F(\bar{X}_-)}{\partial \bar{x}^n} = \sum_{n=1,4,5}\left\langle \frac{f^{\bar{x}^n}(t,\bar{X},\tilde{X})}{|\nabla F(\bar{X})|}\frac{\partial F(\bar{X})}{\partial \bar{x}^n}\right\rangle^{\mathrm{tr}}, \tag{21}$$

where

$$\langle f^{\bar{x}^n}(t,\bar{X},\tilde{X})\rangle = \frac{v_c^3}{\tau_c}\left[\sum_{m=1,4,5}\left(A_{nm}\frac{\partial f_\alpha^0}{\partial \bar{x}^m}\right) + B_n f_\alpha^0\right].$$

This section concludes with a few remarks on the conditions appropriate at the boundaries of phase space. The coefficients A_{nm} and B_n in Eq. (15) vanish at the following boundaries of $\bar{x}^n$: $\gamma_0 = \gamma_{0,\min}$, $v_0 = v_{0,\min}$ (that is, for $v=0$: see Appendix A for the relation between v_0 and v), and $\theta_0 = 0$ and π. This degeneracy leads to the condition that the boundedness of f_α^0 is sufficient, at least for the numerical solution of Eq. (15) (Ref. 5). The boundary condition for $v_0 \to \infty$ depends on the problem under consideration. For many cases,

$$\lim_{v_0\to\infty}\left(A_{4m}\frac{\partial f_\alpha^0}{\partial \bar{x}^m} + B_4 f_\alpha^0\right) = 0$$

is appropriate, although for electron slideaway or runaway situations in tokamaks, for example, another condition should be used.[18] At $\gamma_0 = \gamma_{0,\max}$ a zero or Maxwellian distribution is often a suitable boundary condition.

The initial conditions (at $t=0$) depend on the problem under investigation: it is often natural to take the Maxwellian distribution with appropriate density and temperature profiles.

VI. TOROIDAL CURRENTS AND "RADIAL" FLUXES

Equation (15) may be used to derive the neoclassical fluxes and currents present in a toroidal plasma. For example, it may be used to examine current drive by Ohmic or radio-frequency heating if the appropriate heating terms are added to the equation. Even in the absence of external heating and sources there are inherent neoclassical fluxes and currents in toroidal plasmas, notably the bootstrap current,[13–15,19] and Eq. (15) also allows study of these flows. It should be emphasized that, unlike previous treatments, the neoclassical flows in the presence of distributions that are not close to Maxwellian, including the effects of large banana width and large inverse aspect ratio, may be calculated using Eq. (15). In this section the procedure for calculating the currents and transport fluxes from the distribution $f_\alpha^0(t,\bar{X})$, with $\bar{X}$ the three constants of the motion γ_0, v_0, and θ_0, is described.

The local toroidal current density is

$$j_{\mathrm{tor}}(t,\gamma,\xi) = 2\pi e_\alpha \int_0^\infty \int_0^\pi f_\alpha^0(t,\gamma,\xi,v,\theta) \times \cos\theta\cos\beta\, v^3 \sin\theta\, dv\, d\theta, \tag{22}$$

where $\cos\beta = B_{\mathrm{tor}}/B$, B_{tor} is the toroidal magnetic field and B is the total magnetic field. The total current through the surface labeled γ is given by

$$J_{\mathrm{tor}}(t,\gamma) = \int_{S(\gamma)} j_{\mathrm{tor}}(t,\gamma,\xi)\, ds,$$

where $S(\gamma)$ is the area enclosed by the surface in the poloidal plane.

The procedure for obtaining the radial particle and energy fluxes from the solution of Eq. (15) is now described. The contravariant components of the flux $\bar{\mathbf{j}}$ in the coordinate system $\bar{X}$ come from Eq. (15):

$$\bar{j}^{\bar{x}^n}=\frac{\langle j^{\bar{x}^n}\rangle}{\langle 1\rangle}=\frac{v_c^3}{\tau_c}\frac{1}{\langle 1\rangle}\left[\sum_{m=1,4,5}\left(A_{nm}\frac{\partial f_\alpha^0}{\partial \bar{x}^m}\right)+B_n f_\alpha^0\right].$$

Note that the components of this flux do not vanish for Maxwellian distributions. We require the flux $j_\perp$ through the magnetic surface labeled γ (and not through the drift surface), that is in the direction of the unit vector $\mathbf{n}$ perpendicular to the magnetic surface. This is given by

$$j_\perp=\bar{\mathbf{j}}\cdot\mathbf{n}=\sum_{n=1,4,5}\frac{\partial\gamma}{\partial\bar{x}^n}\frac{\bar{j}^{\bar{x}^n}}{|\nabla\gamma|}.$$

"Radial" particle and energy fluxes may be derived by integration of $j_\perp$ over phase space with appropriate weights. The outward flux of particles through the surface of the torus labeled γ is

$$\Gamma(t,\gamma)=-(2\pi)^2\int_{-\pi}^{\pi}d\xi\int_0^\infty dv\int_0^\pi d\theta\, j_\perp\sqrt{g} \tag{23}$$

and the flux of energy through the same surface is

$$Q(t,\gamma)=-(2\pi)^2\int_{-\pi}^{\pi}d\xi\int_0^\infty dv\int_0^\pi d\theta\,\frac{m_\alpha v^2}{2}\,j_\perp\sqrt{g}, \tag{24}$$

with $\sqrt{g}$ the Jacobian of the transformation from Cartesian to x coordinates.

Equations (23) and (24) give approximate expressions for Γ and Q. More rigorously, one can calculate $j_\perp$ with $O(\tau/\tau_c)$ accuracy using $\mathbf{j}(f_\alpha)$ from Eq. (4) with f_α approximated by f_α^0:

$$j_\perp=\mathbf{j}\cdot\mathbf{n}=\sum_{n=1,2,4,5}\frac{\partial\gamma}{\partial\bar{x}^n}\frac{j^{\bar{x}^n}(f_\alpha^0)}{|\nabla\gamma|},$$

which leads to more complicated expressions for the "radial" fluxes. However, the error in using Eq. (23) is given by

$$2\pi\int_0^\infty dv\int_0^\pi d\theta\left(\sum_{n=1,2,4,5}\int_{-\pi}^{\pi}\frac{\partial\gamma}{\partial\bar{x}^n}\int_0^{2\pi}j^{\bar{x}^n}\,d\varphi\,\frac{\sqrt{g}}{|\nabla\gamma|}\,d\xi\right.$$
$$\left.-2\pi\sum_{n=1,4,5}\int_{-\pi}^{\pi}\frac{\partial\gamma}{\partial\bar{x}^n}\bar{j}^{\bar{x}^n}\frac{\sqrt{g}}{|\nabla\gamma|}\,d\xi\right),$$

and can be small, for example, when there is a dominant term in the summation with $\int_0^{2\pi}j^{\bar{x}^n}\,d\varphi$ close to $2\pi\bar{j}^{\bar{x}^n}$.

VII. NEOCLASSICAL ION FLUXES

In this section we calculate the neoclassical particle and energy fluxes for banana regime ions in a tokamak with circular flux surfaces. We assume that distributions are close to Maxwellian, and that deviations of trajectories from flux surfaces and the inverse aspect ratio $\epsilon=\gamma/R$ are small, so that the fluxes derived can be compared with previous results.[14,15] Unlike previous treatments, however, we do not need to solve a kinetic equation for the perturbation to the distribution, but simply calculate the integrals in Eqs. (23) and (24) using the Maxwellian distribution.

The local radial particle flux for ions is obtained from Eq. (23) by omitting the integrals over toroidal and poloidal angles:

$$\Gamma_i=-2\pi\int_0^\infty dv\int_{\theta_{\rm TPB}^{(1)}}^{\theta_{\rm TPB}^{(2)}}d\theta\, j_\perp\, v^2\sin\theta. \tag{25}$$

The pitch-angle integral has been restricted to trapped particles as, to lowest order in ϵ, the flux of passing particles is zero.[14] For small deviations from flux surfaces $j_\perp$ simplifies to

$$j_\perp\approx\frac{v_c^3}{\tau_c}\frac{A_{11}}{\langle 1\rangle}\frac{\partial f_{\rm M}}{\partial\gamma_0},$$

where the Maxwellian distribution is

$$f_{\rm M}=\left(\frac{m_i}{2\pi T_i}\right)^{3/2}n_i\exp\left(-\frac{m_i v^2}{2T_i}\right), \tag{26}$$

with the density n_i and temperature T_i taken to be functions of the radial coordinate γ only and subscript i denoting the ion species. (The coefficients A_{14} and B_1 give zero contributions after integration over θ, and the A_{15} coefficient multiplies $\partial f/\partial\theta$, which is zero for a Maxwellian.) We now calculate the collisional radial diffusion coefficient $A_{11}/\langle 1\rangle$ assuming no other ion species and neglecting ion–electron collisions, which, to lowest order in m_e/m_i, do not affect the flux.[15] Using Eqs. (3) and (12) we find

$$\frac{A_{11}}{\langle 1\rangle}=-\frac{4\pi Z_i^2}{n_c}\left\langle\frac{\partial\bar{x}^1}{\partial x^l}\frac{\partial\bar{x}^1}{\partial x^m}\frac{\partial x^l}{\partial v_j}\frac{\partial x^m}{\partial v_k}\frac{\partial^2\psi_{\rm ion}}{\partial v_j\partial v_k}\right\rangle\frac{1}{\langle 1\rangle}. \tag{27}$$

For isotropic distributions the Rosenbluth potentials depend only on speed[17,5] and Eq. (27) simplifies to

$$\frac{A_{11}}{\langle 1\rangle}=-\frac{4\pi Z_i^2}{n_c}\left\langle\left(\frac{\partial\gamma_0}{\partial v}\right)^2\frac{d^2\psi_{\rm ion}}{dv^2}+\left(\frac{\partial\gamma_0}{\partial\theta}\right)^2\frac{1}{v^3}\frac{d\psi_{\rm ion}}{dv}\right\rangle\frac{1}{\langle 1\rangle}.$$

For Maxwellian distributions,[5]

$$\frac{d\psi_{\rm ion}}{dv}=-\frac{n_i}{4\pi^{3/2}}y(u),$$

$$y(u)\equiv\frac{1}{2u}e^{-u^2}+\left(2-\frac{1}{u^2}\right)\frac{\sqrt{\pi}}{4}\,{\rm erf}(u),$$

where

$${\rm erf}(u)=\frac{2}{\sqrt{\pi}}\int_0^u e^{-s^2}ds$$

is the error function, $v_i=(2T_i/m_i)^{1/2}$ is the thermal speed, and $u=v/v_i$. Introducing the poloidal Larmor radius, $\rho_p=m_iv_i/(Z_i|e|B_p)$ with B_p the poloidal field, and remembering that γ_0 for trapped particles is the flux surface radius at the banana tip, it is straightforward to show that (cf. Appendix A)

$$\frac{\partial\gamma_0}{\partial v}=-\frac{\rho_p\cos\theta}{v_i}$$

and

$$\frac{\partial\gamma_0}{\partial\theta}=u\rho_p\sin\theta.$$

These give

$$\frac{A_{11}}{\langle 1\rangle}=-\frac{4\pi Z_i^2\rho_p^2}{n_c}\left(\frac{\cos^2\theta}{v_i^2}\frac{d^2\psi_{\rm ion}}{dv^2}+u^2\sin^2\theta\frac{1}{v^3}\frac{d\psi_{\rm ion}}{dv}\right),$$

where $\langle 1\rangle$ has canceled on the right-hand side. For circular flux surfaces we have $\cos\theta_{\rm TPB}\simeq\pm\sqrt{\epsilon(1+\cos\xi)}$ [from the tokamak field $\propto 1/(1+\epsilon\cos\xi)$], giving

$$\int_{\theta_{\rm TPB}^{(1)}}^{\theta_{\rm TPB}^{(2)}}\cos^2\theta\sin\theta\,d\theta=O(\epsilon^{3/2})$$

and

$$\int_{\theta_{\rm TPB}^{(1)}}^{\theta_{\rm TPB}^{(2)}}\sin^3\theta\,d\theta\approx 2\sqrt{\epsilon(1+\cos\xi)}.$$

Retaining only terms $O(\epsilon^{1/2})$ in Γ_i gives

$$\Gamma_i=\frac{16\pi^2 Z_i^2\rho_p^2 v_c^3\epsilon^{1/2}}{n_c\tau_c}\int_0^\infty dv\,\frac{\partial f_{\rm M}}{\partial\gamma_0}\frac{u^2}{v}\frac{d\psi_{\rm ion}}{dv}.$$

This reduces to

$$\Gamma_i=-\frac{3}{\pi^{1/2}}\nu_{ii}\rho_p^2\epsilon^{1/2}n_i\left[\left(\frac{1}{n_i}\frac{dn_i}{d\gamma}+\frac{Z_i|e|}{T_i}\frac{d\Phi}{d\gamma}\right)I_1+\frac{1}{T_i}\frac{dT_i}{d\gamma}\left(I_3-\frac{3}{2}I_1\right)\right],\tag{28}$$

where

$$I_n=\int_0^\infty y(u)u^n e^{-u^2}\,du,$$

and we have introduced the ion–ion collision frequency,

$$\nu_{ii}=\frac{16\pi^{1/2}n_i Z_i^4 e^4\ln\Lambda}{3(4\pi\epsilon_0)^2 m_i^2 v_i^3},$$

for easy comparison with results in Ref. 15. The term involving $d\Phi/d\gamma$ in Eq. (28) comes from the $(\partial v/\partial\gamma_0)\partial f_{\rm M}/\partial v$ term in $\partial f_{\rm M}/\partial\gamma_0$ using $v_0^2=v^2+2Z_i|e|\Phi/m_i$, and taking the electrostatic potential Φ a function of radius but not poloidal angle.[14]

A very similar calculation gives the local ion heat flux Q_i,

$$Q_i=-\frac{3}{\pi^{1/2}}\nu_{ii}\rho_p^2\epsilon^{1/2}n_iT_i\left[\left(\frac{1}{n_i}\frac{dn_i}{d\gamma}+\frac{Z_i|e|}{T_i}\frac{d\Phi}{d\gamma}\right)I_3+\frac{1}{T_i}\frac{dT_i}{d\gamma}\left(I_5-\frac{3}{2}I_3\right)\right].$$

Numerical calculations give $I_1=0.2361$, $I_3=0.3133$, and $I_5=0.7050$. Thus

$$\Gamma_i=-\nu_{ii}\rho_p^2\epsilon^{1/2}n_i\left[0.40\left(\frac{1}{n_i}\frac{dn_i}{d\gamma}+\frac{Z_i|e|}{T_i}\frac{d\Phi}{d\gamma}\right)-0.07\frac{1}{T_i}\frac{dT_i}{d\gamma}\right]\tag{29}$$

and

$$Q_i=-\nu_{ii}\rho_p^2\epsilon^{1/2}n_iT_i\left[0.53\left(\frac{1}{n_i}\frac{dn_i}{d\gamma}+\frac{Z_i|e|}{T_i}\frac{d\Phi}{d\gamma}\right)I_3+0.40\frac{1}{T_i}\frac{dT_i}{d\gamma}\right].\tag{30}$$

The four coefficients, 0.40, −0.07, 0.53, and 0.40, agree with the values 0.39, −0.07, 0.52, and 0.40 obtained by ignoring the second ion species in Eqs. (48) and (52) of Ref. 15. The small differences are due to the equivalents of I_n in Ref. 15 being given to only two decimal places. However, it is known that self-collisions [used to derive Eqs. (29) and (30)] do not lead to a net particle flux, because they conserve momentum [see, for example, Eq. (27) in Ref. 15]. Thus the radial electric field $-d\Phi/d\gamma$ adjusts to ensure that $\Gamma_i=0$ (this effect is discussed in Sec. VI C 2 of Ref. 14 and in detail in Ref. 20). Using the resulting expression for $d\Phi/d\gamma$ gives

$$Q_i=-0.49\nu_{ii}\rho_p^2\epsilon^{1/2}n_i\frac{dT_i}{d\gamma}.\tag{31}$$

Thus we have derived the neoclassical ion heat flux for the banana regime, Eq. (31), a result identical with that derived by other authors.[14,15] This did not require the solution of a kinetic equation, unlike previous derivations, and helps confirm the validity of Eq. (15).

VIII. CONCLUSIONS

In this paper a procedure for deriving the neoclassical low collisionality nonlinear 3-D kinetic equation (more precisely, a set of equations) has been described. The procedure allows arbitrary deviations of particle trajectories from flux surfaces and the distribution functions satisfying the resulting equations, which need not be close to Maxwellian, yield toroidal currents and "radial" transport fluxes. The Coulomb collision term has been treated using this procedure, together with axisymmetry and the drift approximation for particle motion, to derive Eq. (15). The coefficients of this equation have been given in a form convenient for numerical evaluation. Derivation of the appropriate operators for other relevant effects (particle source terms, additional heating, magnetic field ripple, and other transport mechanisms, etc.) using the technique described in Sec. III is possible if a choice of "slow" and "fast" variables that describes particle trajectories allowing for the relevant physics can be made. Work in this direction is in progress.

Ideally, one should solve for the distributions of electrons and all ion species using the currents derived to give a self-consistent magnetic field $\mathbf{B}(\gamma,\xi)$ and imposing quasineutrality to determine the electrostatic potential $\Phi(\gamma,\xi)$. In practice, it would be more tractable to impose equilibrium fields and potentials and solve for one species only, assuming implicitly that the behavior of the other species maintains these fields and potentials.

We have shown that neoclassical particle and energy fluxes for Maxwellian ions may be calculated without a solution of the equation, and our results [Eqs. (29)–(31)] agree with those of other authors. For more complicated problems involving strongly non-Maxwellian distributions and/or large banana widths solutions to Eq. (15) are required. Analytic methods are unlikely to provide these and so computer solutions are necessary. A simplified version of this equation, which contained only the neoclassical radial diffusion coefficient, has already been solved numerically.[21] The results of this calculation were consistent with analytic results and with 2-D calculations. Programs for calculation of all the coefficients appearing in Eq. (15) have been written and a solution of Eq. (15) with appropriate boundary conditions is planned. This should allow calculation of neoclassical flows associated with large deviations from flux surfaces and with non-Maxwellian distributions, two features of alpha particles in reactors for example.

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APPENDIX A: CONSTANTS OF DRIFT MOTION

The constants of motion γ_0, v_0, and θ_0 come from the three integrals of the system of ordinary differential equations, which describes drift motion of charged particles in axisymmetric collisionless toroidal plasmas.[16] These integrals gives conservation of the magnetic moment,

$$\frac{mv^2 \sin^2\theta}{2B(\gamma,\xi)} = \text{const},$$

conservation of total particle energy in stationary magnetic and electric fields,

$$\frac{mv^2}{2} + e_\alpha \Phi(\gamma,\xi) = \text{const},$$

and conservation of generalized toroidal momentum,

$$mv\sqrt{g_{33}^{\text{real}}}\cos\theta\cos\beta - e_\alpha\psi(\gamma) = \text{const}.$$

Here

$$\psi(\gamma) = \int \sqrt{g^{\text{real}}}\,\frac{B_{\text{pol}}}{\sqrt{g_{22}^{\text{real}}}}\,d\gamma$$

is the poloidal flux; B_{pol} is the poloidal magnetic field; $\sqrt{g^{\text{real}}}$ is the Jacobian of the real space coordinate system (γ,ξ,η); g_{22}^{real} and g_{33}^{real} are the components of the metric tensor in real space; $\cos\beta = B_{\text{tor}}/B$ with B_{tor} the toroidal field; and $\Phi(\gamma,\xi)$ is the electrostatic potential.

Different choices for γ_0, v_0, and θ_0 may be made by appropriate selection of the right-hand sides in the above expressions. A convenient choice is as follows: γ_0 is the flux surface label on the inside of the drift trajectory for passing particles and at the bounce points for trapped particles, v_0 is the speed corresponding to the total energy, and θ_0 is the pitch angle at the outermost point of the drift trajectory. The dependence of γ_0, v_0, and θ_0 on the local coordinates x is given by a system of seven transcendental algebraic equations,

$$\begin{aligned}\frac{mv_0^2}{2} &= \frac{mv^2}{2} + e_\alpha\Phi(\gamma,\xi)\\ &= \frac{m(v^o)^2}{2} + e_\alpha\Phi(\gamma^o,0)\\ &= \frac{m(v^i)^2}{2} + e_\alpha\Phi(\gamma_0,\xi^i),\end{aligned} \tag{A1}$$

$$\frac{mv^2\sin^2\theta}{2B(\gamma,\xi)} = \frac{m(v^o)^2\sin^2\theta_0}{2B(\gamma^o,0)} = \frac{m(v^i)^2\sin^2\theta^i}{2B(\gamma_0,\xi^i)}, \tag{A2}$$

and

$$\begin{aligned}&mv\sqrt{g_{33}^{\text{real}}(\gamma,\xi)}\cos\theta\cos\beta(\gamma,\xi) - e_\alpha\psi(\gamma)\\ &\quad= mv^o\sqrt{g_{33}^{\text{real}}(\gamma^o,0)}\cos\theta_0\cos\beta(\gamma^o,0) - e_\alpha\psi(\gamma^o)\\ &\quad= mv^i\sqrt{g_{33}^{\text{real}}(\gamma_0,\xi^i)}\cos\theta^i\cos\beta(\gamma_0,\xi^i) - e_\alpha\psi(\gamma_0).\end{aligned} \tag{A3}$$

In Eqs. (A1)–(A3), γ^o is the flux surface label on the outside and θ^i is the pitch angle on the inside of the drift trajectory, with $\theta^i = \pi/2$ for trapped particles; v^o and v^i are the speeds at the outside and inside of the trajectory; ξ^i is the poloidal angle at reflection for trapped particles and π for passing particles. For trapped particles there is indeterminacy in some of these definitions, particularly if the plasma is not up–down symmetric. A convenient choice is to take γ_0, v^i, and ξ^i for the upper reflection point, and $\theta_0 < \pi/2$, which fixes γ^o. Formulas for $\partial\bar{x}^n/\partial x^l$ and $\partial x^l/\partial\bar{x}^n$ can then be obtained from these seven transcendental equations and used to calculate the Jacobian and the metric coefficients.

If the following assumptions are valid, then analytic formulas can be found for the dependence of $\bar{x}(x)$ and $x(\bar{x})$ by Taylor expansion of $\psi(\gamma^0) - \psi(\gamma)$:

$$\frac{|\gamma_0-\gamma|}{R} \ll 1, \quad \left(\frac{\gamma_0-\gamma}{\gamma_a}\right)^2 \ll 1, \quad B \gg \frac{\partial B}{\partial\gamma}|\gamma_0-\gamma|.$$

Here R is the major radius and γ_a is the minor radius.

APPENDIX B: FORMULAS FOR $\bar{U}_{lj}$ and $\bar{U}'_{lj}$

After much algebra one can show that the matrix elements $\bar{U}_{lj}, \bar{U}'_{lj}$ in Sec. IV can be expressed in terms of complete elliptical integrals:

$$\begin{aligned}\bar{U}_{44} = 2\pi\{&I_1 - I_2(v - v'\cos\theta\cos\theta')^2 + v'\sin\theta\sin\theta'\\ &\times[2I_3 v - v'(I_4\sin\theta\sin\theta' + 2I_3\cos\theta\cos\theta')]\},\end{aligned}$$

$$\begin{aligned}\bar{U}_{55} = \frac{2\pi}{v^2}\{&I_1 - v'[\sin\theta\cos\theta'(I_2\sin\theta\cos\theta'\\ &-2I_3\cos\theta\sin\theta') + I_4\cos^2\theta\sin^2\theta']\},\end{aligned}$$

$$\bar{U}_{66} = \frac{2\pi}{v^2\sin^2\theta}(I_1 - I_5 v'^2\sin^2\theta'),$$

$$\bar{U}_{45}=\bar{U}_{54}=-2\pi\{v'(I_2\sin\theta\cos\theta'-I_3\cos\theta\sin\theta')$$
$$-\frac{v'^2}{v}[I_3(\sin^2\theta-\cos^2\theta)\sin\theta'\cos\theta'$$
$$+\sin\theta\cos\theta(I_2\cos^2\theta'-I_4\sin^2\theta')]\},$$

$$\bar{U}_{46}=\bar{U}_{64}=\bar{U}_{56}=\bar{U}_{65}=0,$$

$$\bar{U}'_{44}=2\pi\{I_1\cos\theta\cos\theta'+I_6\sin\theta\sin\theta'$$
$$+I_2[vv'-\cos\theta\cos\theta'$$
$$\times(v'^2+v^2-vv'\cos\theta\cos\theta')]-I_3\sin\theta\sin\theta'$$
$$\times(v'^2+v^2-2vv'\cos\theta\cos\theta')$$
$$+I_4vv'\sin^2\theta\sin^2\theta'\},$$

$$\bar{U}'_{55}=2\pi[(I_1\sin\theta\sin\theta'+I_6\cos\theta\cos\theta')/(vv')$$
$$+(I_2+I_4)\sin\theta\cos\theta\sin\theta'\cos\theta'$$
$$-I_3(\cos^2\theta\sin^2\theta'+\sin^2\theta\cos^2\theta')],$$

$$\bar{U}'_{66}=2\pi\left(\frac{I_6}{vv'\sin\theta\sin\theta'}-I_5\right),$$

$$\bar{U}'_{45}=2\pi\{(I_6\sin\theta\cos\theta'-I_1\cos\theta\sin\theta')/v'$$
$$+v[v(I_2\sin\theta'\cos\theta-I_3\cos\theta'\sin\theta)/v'$$
$$+\sin\theta'\cos\theta'(I_4\sin^2\theta-I_2\cos^2\theta)$$
$$+I_3\sin\theta\cos\theta(\cos^2\theta'-\sin^2\theta')]\},$$

$$\bar{U}'_{54}=2\pi\{(I_6\sin\theta'\cos\theta-I_1\cos\theta'\sin\theta)/v$$
$$+v'[v'(I_2\sin\theta\cos\theta'-I_3\cos\theta\sin\theta')/v$$
$$+\sin\theta\cos\theta(I_4\sin^2\theta'-I_2\cos^2\theta')$$
$$+I_3\sin\theta'\cos\theta'(\cos^2\theta-\sin^2\theta)]\},$$

$$\bar{U}'_{46}=\bar{U}'_{64}=\bar{U}'_{56}=\bar{U}'_{65}=0,$$

where

$$I_1=\frac{4}{\sqrt{a}}\frac{1}{\sqrt{1+p^2}}F,$$

$$I_2=\frac{4}{a^{3/2}}\frac{1}{\sqrt{1+p^2}}E,$$

$$I_3=\frac{4}{a^{3/2}}\frac{1}{p^2\sqrt{1+p^2}}[(2+p^2)E-2F],$$

$$I_4=I_2-I_5,$$

$$I_5=\frac{16}{a^{3/2}}\frac{1}{p^4\sqrt{1+p^2}}[(2+p^2)F-2(1+p^2)E],$$

$$I_6=\frac{4}{\sqrt{a}}\frac{1}{p^2\sqrt{1+p^2}}[(2+p^2)F-2(1+p^2)E].$$

Here

$$a=v^2-2vv'\cos(\theta'-\theta)+v'^2,$$

$$b=4vv'\sin\theta\sin\theta',\quad p=\sqrt{b/a},$$

and $F(k)$ and $E(k)$ are complete elliptical integrals of the first and the second kind with $k=p/\sqrt{1+p^2}$. For $p=0$, $I_3\cdots I_6$ reduce to $I_4=I_5=\pi/a^{3/2}$, $I_3=I_6=0$.

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