Neoclassical Transport Including Collisional Nonlinearity

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In the standard δf theory of neoclassical transport, the zeroth-order (Maxwellian) solution is obtained analytically via the solution of a nonlinear equation. The first-order correction δf is subsequently computed as the solution of a linear, inhomogeneous equation that includes the linearized Fokker-Planck collision operator. This equation admits analytic solutions only in extreme asymptotic limits (banana, plateau, Pfirsch-Schlüter), and so must be solved numerically for realistic plasma parameters. Recently, numerical codes have appeared which attempt to compute the total distribution f more accurately than in the standard ordering by retaining some nonlinear terms related to finite-orbit width, while simultaneously reusing some form of the linearized collision operator. In this work we show that higher-order corrections to the distribution function may be unphysical if collisional nonlinearities are ignored.

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While neoclassical transport is generally subdominant to drift-wave-driven turbulent transport in the tokamak core, neoclassical transport can become important in the H-mode edge transport barrier region and in internal transport barriers, where turbulence is suppressed, and in the near axis region, where the temperature and density gradients become small. In both cases, nonlocal effects, which are not retained in the standard theory [\[1\]](#page-3-1), are believed to play an important role in the transport dynamics. Specifically, in a transport barrier, the characteristic short temperature and density gradient length scales can be comparable to the ion poloidal gyroradius, while near the magnetic axis, trapped particles follow potato orbits, for which the orbit width becomes comparable to or larger than the minor radius. Over the past decade there have been attempts to use direct numerical simulation to describe nonlocal and other effects [[2\]](#page-3-2). Numerical codes (of both the gyrokinetic [[3\]](#page-3-3) and neoclassical [[4](#page-3-4),[5\]](#page-3-5) type) have appeared with the aim of computing a more accurate solution than that described by the standard δf model [[6\]](#page-3-6). While there are advanced analytic treatments relevant to, for example, the plasma flow in the H -mode pedestal [[7](#page-3-7)] as well as the gyrokinetic treatment of toroidal angular momentum transport [\[8\]](#page-3-8), no consensus regarding a suitable systematic formalism appropriate for numerical simulation has emerged. In fact, the numerical simulations may sometimes ignore key terms that are retained in the analytic theories. Although there is not, at this time, a standard generalization of the local theory relevant for numerical simulation, a representative starting point in the neoclassical limit is the well-known Hazeltine equation [[9\]](#page-3-9) for the total ion distribution f :

$$
\frac{df}{dt} + \mathbf{v}_g \cdot \nabla f + \dot{\mu} \frac{\partial f}{\partial \mu} = C(f, f). \tag{1}
$$

Above, v_g is the general guiding-center velocity which includes both perpendicular and parallel drifts. The gradient is taken at constant total energy $E = v^2/2 +$ $z_i e \Phi_0/m_i$. In these expressions, C is the nonlinear Fokker-Planck collision operator, v is the particle velocity, Φ_0 is the equilibrium-scale electrostatic potential, z_i is the ion charge, and m_i is the mass of the primary ion species. There appears to be a tacit consensus that Eq. [\(1\)](#page-0-0) forms a sufficiently accurate model for nonlocal dynamics because it includes so-called finite-orbit effects through the advective term $\mathbf{v}_g \cdot \nabla f$ [[10](#page-3-10),[11](#page-3-11)]. And, importantly, the left-hand side of Eq. [\(1](#page-0-0)) was shown by Hinton [\[12\]](#page-3-12) to be exactly conservative—insofar as it can be transformed to an exact phase-space gradient. This feature is often considered advantageous for numerical simulation. On the other hand, the complexity of the full nonlinear collision operator in Eq. ([1](#page-0-0)) is such that all existing research groups take a pragmatic approach and replace it with some model form of the linearized operator $C_L(f)$. Indeed, even the test-particle part of C_L is so complicated that the numerical codes referred to above implement it in model [\[13\]](#page-3-13), rather than exact [[14](#page-3-14)], form.

Calculations by Simakov and Catto [\[15\]](#page-3-15) in the limit of short mean-free path, however, show that corrections to the Hazeltine equation (which is valid to all orders in the poloidal gyroradius ρ_{ip}) appear at second order in the ion gyroradius ρ_i . Even so, the Simakov model has not been the focus of any simulation work. Presumably, this has happened because full-f research attempts to extend the accuracy of local calculations to include higher-order poloidal gyroradius corrections. In this regime, poloidal ion gyroradius over scale-length deviations from a local Maxwellian equilibrium are possible. However, if accurate corrections to the local theory are of interest, then the common practice of linearizing C is incorrect. It is the repercussions of using only a linearized collision operator in the Hazeltine model that is the focus of the remainder of this work. Coupling to electrons and impurities is ignored to focus on the nonlinear effect of concern.

Perturbative hierarchy.—The Hazeltine equation for the total f is intractable in toroidal geometry. Still, asymptotic consistency requires that as $\rho_{ip}/a \rightarrow 0$, the exact solution f must satisfy

$$
f - f_0 - f_1 - \dots - f_N \to 0,
$$
 (2)

where f_N is the Nth term in the expansion of f in powers of ρ_{ip}/a . By considering the steady-state limit, and under the further simplifying assumption that the potential $\Phi =$ $\Phi_0(r)$ is a flux function [\[16](#page-3-16)], a series expansion in powers of ρ_{in}/a yields the hierarchy

$$
v_{\parallel} \mathbf{b} \cdot \nabla f_0 - C(f_0, f_0) = 0, \tag{3}
$$

$$
v_{\parallel} \mathbf{b} \cdot \nabla f_1 - C_L(f_1) = \mathcal{L}_v f_0, \tag{4}
$$

$$
v_{\parallel} \mathbf{b} \cdot \nabla f_2 - C_L(f_2) - C(f_1, f_1) = \mathcal{L}_v f_1,\tag{5}
$$

where \mathcal{L}_v is the differential operator

$$
\mathcal{L}_v \doteq -\mathbf{v}_D \cdot \nabla + \mathbf{v}_E^{(0)} \cdot \nabla + \frac{z_i e}{m_i} \mathbf{v}_D \cdot \nabla \Phi_0 \frac{\partial}{\partial \varepsilon} - \dot{\mu} \frac{\partial}{\partial \mu}.
$$
 (6)

In contrast to Eq. [\(1](#page-0-0)), we have evaluated gradients at constant kinetic energy $\varepsilon = v^2/2$. To keep the details as simple as possible, we use the low- β approximation, $\left(\frac{a}{B^2}\right)\left|\frac{dp}{dr}\right| \ll 1$, to write [[17](#page-3-17)]

$$
\mathbf{v}_E^{(0)} \cdot \nabla \theta = \frac{I}{\psi'} \frac{c}{\mathcal{J}_\psi B^2} \Phi'_0,\tag{7}
$$

$$
\mathbf{v}_D \cdot \nabla r = -\frac{I}{\psi'} \frac{v_{\parallel}^2 + \mu B}{\Omega B} \frac{1}{\mathcal{J}_{\psi} B} \frac{\partial B}{\partial \theta},\tag{8}
$$

$$
\mathbf{v}_D \cdot \nabla \theta = \frac{I}{\psi'} \frac{v_{\parallel}^2 + \mu B}{\Omega B} \frac{1}{\mathcal{J}_{\psi} B} \frac{\partial B}{\partial r} - \frac{I'}{\psi'} \frac{\mu B}{\Omega B} \frac{1}{\mathcal{J}_{\psi}}, \quad (9)
$$

$$
v_{\parallel} \mathbf{b} \cdot \nabla \theta = \frac{v_{\parallel}}{\mathcal{J}_{\psi} B},\tag{10}
$$

$$
\dot{\mu} = -\mu \mathbf{v}_D \cdot \nabla r \frac{I'}{I}.
$$
\n(11)

Above, μ is the magnetic moment, $\Omega = z_i e B/(m_i c)$ is the ion cyclotron frequency, ψ is the poloidal flux divided by 2π , $\mathbf{b} = \mathbf{B}/B$,

$$
\mathbf{B} = \nabla \varphi \times \nabla \psi + I \nabla \varphi, \tag{12}
$$

and $\mathcal{J}_{\psi} = (\nabla \psi \times \nabla \theta \cdot \nabla \varphi)^{-1}$. *C* is the like-species (nonlinear) collision operator, which can be written in Landau [\[18\]](#page-3-18) form as

$$
C(f,g) = -L_{ii} \frac{\partial}{\partial v_k} \int d^3 v' U_{kl} \bigg[f(\mathbf{v}) \frac{\partial g(\mathbf{v}')}{\partial v'_l} - g(\mathbf{v}') \frac{\partial f(\mathbf{v})}{\partial v_l} \bigg],
$$
\n(13)

where $U_{kl} = (u^2 \delta_{kl} - u_k u_l)/u^3$, $u_k = v_k - v'_k$, and $L_{ii} =$ $4\pi z_i^2 e^4 \ln \Lambda / m_i^2$. In Eqs. [\(4\)](#page-1-0) and [\(5\)](#page-1-1), $C_L(g) = C(g, f_0) +$ $C(f_0, g)$ is the linearized collision operator. Noting that $U_{kl}u_l = 0$, it is easy to show directly from Eq. [\(13\)](#page-1-2) that $C(f_0, f_0) = 0$, where f_0 is a local Maxwellian:

$$
f_0 = \frac{n(r)}{[2\pi T(r)/m_i]^{3/2}} e^{-m_i \varepsilon/T(r)}.
$$
 (14)

By inspection, it is clear that the solution of Eq. [\(3\)](#page-1-3) is also a Maxwellian. Proceeding to Eq. ([4](#page-1-0)) for the first-order distribution f_1 , we insert the solution for f_0 to obtain

$$
v_{\parallel} \mathbf{b} \cdot \nabla f_1 - C_L(f_1) = \mathbf{v}_D \cdot \nabla r \bigg[-\frac{\partial f_0}{\partial r} - \frac{e}{T} \frac{\partial \Phi_0}{\partial r} f_0 \bigg]. \tag{15}
$$

This equation represents the standard model for neoclassical transport and cannot be solved analytically in the general case.

Exact solution for f_1 .—An important limit, for which an exact first-order solution exists, is the case of a single ion species with uniform temperature. By noting the identity

$$
\mathbf{v}_D \cdot \nabla r = \frac{I}{\psi'} v_{\parallel} \mathbf{b} \cdot \nabla \left(\frac{v_{\parallel}}{\Omega}\right),\tag{16}
$$

and assuming zero temperature gradient, we can reduce Eq. (15) (15) (15) to

$$
v_{\parallel} \mathbf{b} \cdot \nabla f_1 - C_L(f_1) = v_{\parallel} \mathbf{b} \cdot \nabla \left(\frac{v_{\parallel}}{\Omega}\right) F(r, \varepsilon), \qquad (17)
$$

where

$$
F(r,\,\varepsilon) \doteq -\frac{I}{\psi'} \bigg(\frac{d \ln n}{dr} + \frac{z_i e \Phi_0'}{T} \bigg) f_0. \tag{18}
$$

The solution of this equation is simply the first-order part of the low-flow drifting Maxwellian,

$$
f_1 = \left(\frac{v_{\parallel}}{\Omega}\right) F(r, \varepsilon). \tag{19}
$$

To obtain this result we have used $C_l(f_0v_{\parallel}) = 0$, which reflects momentum conservation. While the first-order solution is independent of the collisional regime, the higherorder solutions are not.

Asymptotic solution for f_2 . Some algebra shows that Eq. [\(5](#page-1-1)) reduces exactly to the following relatively compact inhomogeneous equation for f_2 :

$$
v_{\parallel} \mathbf{b} \cdot \nabla (f_2 - \tilde{f}_2) = C_L(f_2) + C(f_1, f_1), \qquad (20)
$$

where

$$
\tilde{f}_2 = -\frac{1}{2} \left(\frac{v_{\parallel}}{\Omega}\right)^2 G(r, \varepsilon).
$$
 (21)

Here, G is the profile function

$$
G(r,\varepsilon) = \frac{I}{\psi'} \left(\frac{\partial F}{\partial r} + \frac{z_i e \Phi_0'}{T} F \right).
$$
 (22)

The function G will appear as a driving term in the solution in all collisional regimes, the banana and Pfirsch-Schlüter regimes in particular. The (perturbative) nonlocal character of the solution is evident in the second derivatives appearing in G. To obtain the solution in the limit $L_{ii} \rightarrow 0$, we see by inspection that

$$
f_2 - \tilde{f}_2 = g_2(\varepsilon, \mu, \sigma, r) + \mathcal{O}(L_{ii}), \tag{23}
$$

where g_2 is an integration constant which is determined by the appropriate solvability condition. Although g_2 is independent of the poloidal angle θ , it may in principle depend on the sign of velocity, $\sigma = |v_{\parallel}|/v_{\parallel}$.

Solvability with linear collisions.—First we examine the case for which only the linearized collision operator C_L is retained. Then, the solvability condition takes the form

$$
\oint \frac{d\theta}{v_{\parallel}} \mathcal{J}_{\psi} BC_L(f_2) = 0. \tag{24}
$$

We can write this symbolically as

$$
\left\langle \frac{B}{v_{\parallel}} C_L(f_2) \right\rangle = 0, \tag{25}
$$

where the angle brackets denote a flux-surface average.

Solvability with nonlinear collisions.—On the other hand, if the nonlinear collision operator is properly accounted for, then the solvability condition takes the form

$$
\left\langle \frac{B}{v_{\parallel}} (C_L(f_2) + C(f_1, f_1)) \right\rangle = 0.
$$
 (26)

At this point, we note the identity

$$
C(f_0 v_k, f_0 v_k) = -\frac{1}{2} C_L(v_k^2 f_0), \qquad (27)
$$

which can be proved directly from the Landau form of the like-particle operator, Eq. [\(13\)](#page-1-2). Remarkably, this allows us to express the nonlinear solvability condition completely in terms of the linearized operator

$$
\left\langle \frac{B}{v_{\parallel}} C_L \left(f_2 - \frac{1}{2} \frac{v_{\parallel}^2}{\Omega^2} \frac{F^2}{f_0} \right) \right\rangle = 0.
$$
 (28)

Symbolic solution.—The solution of an equation of the form

$$
\left\langle \frac{B}{v_{\parallel}} C_{L}[g(\varepsilon, \mu, \sigma, r) - \Lambda(\varepsilon, \mu, \sigma, r, \theta)] \right\rangle = 0 \quad (29)
$$

can be written as $g(\varepsilon, \mu, \sigma, r) = \overline{\Lambda}$, where the overbar denotes a linear transformation which corresponds roughly to a flux-surface average. More precisely, we refer to Λ as the *collisional average* of Λ . Computing this transform exactly is analytically intractable in the general case. Still, using this notation, the solutions f_2^L of Eq. ([25\)](#page-2-0) and f_2^{NL} of Eq. ([28](#page-2-1)) can be written

$$
f_2^L = \frac{1}{2} \left(\frac{v_{\parallel}}{\Omega}\right)^2 G - \frac{1}{2} \left(\frac{v_{\parallel}}{\Omega}\right)^2 G,\tag{30}
$$

$$
f_2^{\text{NL}} = \frac{1}{2} \left(\frac{v_{\parallel}}{\Omega}\right)^2 G - \frac{1}{2} \left(\frac{v_{\parallel}}{\Omega}\right)^2 G + \frac{1}{2} \left(\frac{v_{\parallel}}{\Omega}\right)^2 \frac{F^2}{f_0}.
$$
 (31)

Physically, the two solutions are quite distinct. While the collisional average of f_2^L is zero, the solution including the collisional nonlinearity f_2^{NL} contains a significant contribution from $C(f_1, f_1)$ which does not vanish on collisional average. For clarity, we emphasize that the solutions above apply only to the special case of uniform temperature.

Physical interpretation.—Some insight into the differing solutions can be obtained by examining more closely the form of the function g_2 .

$$
g_2^{\text{NL}} = \frac{1}{2} \left(\frac{v_{\parallel}}{\Omega}\right)^2 \left(G + \frac{F^2}{f_0}\right)
$$
 (32)

$$
= \frac{1}{2} \left(\frac{v_{\parallel}}{\Omega}\right)^2 f_0 \frac{z_i e}{c T_i} \frac{I}{\psi'} \frac{\partial}{\partial r} \langle U_{\parallel} B \rangle, \tag{33}
$$

which shows that only the shear in the parallel velocity, $\langle U_{\parallel} B \rangle = -(cT/e z_i)(I/\psi')(d \ln n/dr + z_i e \Phi_0'/T)$, acts as a drive. Indeed, because of the Galilean invariance of the nonlinear collision operator, a rigidly rotating Maxwellian cannot act as a neoclassical drive. However, if C is approximated by C_L , exactly such an unphysical drive will occur. We also remark that in the absence of parallel velocity shear, the solution reduces to $f_2^{\text{NL}} =$ $(m_i v_{\parallel} \langle U_{\parallel} B \rangle / B T)^2 / 2$, which is just the second-order part of a drifting Maxwellian in the low-flow ordering.

Banana-regime example.—We can give the calculation a more intuitive flavor by carrying out the averaging operation explicitly in the banana regime using the model Kovrizhnikh operator. When acting on an even function of σ , the Kovrizhnikh operator reduces to the pitch-angle scattering (Lorentz) operator

$$
C_L \sim \frac{B}{B_0} \frac{\nu_{\parallel}}{\varepsilon} \frac{\partial}{\partial \lambda} \lambda \nu_{\parallel} \frac{\partial}{\partial \lambda},\tag{34}
$$

with $\lambda = \mu B_0 / \varepsilon$, $v_{\parallel} = \sqrt{2\varepsilon (1 - \lambda B / B_0)}$, such that B_0 is the on-axis magnetic field strength. Some algebra then shows that the solvability condition in the case of the linear operator is

$$
\frac{\partial}{\partial \lambda} \left[-\frac{\partial}{\partial \lambda} \left\langle \frac{1}{3} \frac{v_{\parallel}^{3}}{\Omega^{2}} \right\rangle G + \lambda \langle v_{\parallel} \rangle \frac{\partial g_{2}^{L}}{\partial \lambda} \right] = 0, \quad (35)
$$

or equivalently,

$$
\frac{\partial g_2^L}{\partial \lambda} = \frac{1}{\langle v_{\parallel} \rangle} \frac{\partial}{\partial \lambda} \left\langle \frac{1}{3} \frac{v_{\parallel}^3}{\Omega^2} \right\rangle G. \tag{36}
$$

It is difficult to obtain a useful closed-form solution to this equation in the general case, and so we take the subsidiary limit $\epsilon \rightarrow 0$, in which case it can be shown,

$$
\frac{\partial g_2^L}{\partial \lambda} \sim -\frac{\varepsilon}{\Omega_0^2} G \Bigg(1 + \epsilon \frac{\oint d\theta \mathcal{J}_{\psi} \cos \theta \sqrt{1 - \lambda B/B_0}}{\oint d\theta \mathcal{J}_{\psi} \sqrt{1 - \lambda B/B_0}} \Bigg). \tag{37}
$$

Here, $\Omega_0 = z_i e B_0 / (m_i c)$ is the on-axis cyclotron frequency, $\epsilon = r/R_0$ is the inverse aspect ratio, and R_0 is the plasma major radius. Thus, neglecting terms of order $\epsilon^{3/2}$, we can perform the λ integration directly to show $g_2^L \sim -(\lambda \varepsilon/\Omega_0^2)G + c(\varepsilon, r)$, where c is an integration constant. By choosing the flux-surface average of the density moment to be zero, we can eliminate c to find

$$
f_2^{\rm L} \sim \frac{(-2\varepsilon + \mu B_0)}{\Omega_0^2} G \epsilon \cos \theta. \tag{38}
$$

The accuracy of this result has been verified numerically with the NEO code [[17](#page-3-17)]. We note in passing that a similar result is obtained in the Pfirsch-Schlüter regime even though the details of the calculation are quite different. The similarity, ultimately, arises from properties of the general solvability condition [see Eq. (96) in Ref. [\[17](#page-3-17)]], which invariably removes a weighted θ average of the inhomogeneous terms.

Next, the same formal procedure, when applied to the case of the full nonlinear operator, gives the significantly different result

$$
f_2^{\text{NL}} \sim \frac{(-2\varepsilon + \mu B_0)}{\Omega_0^2} G \epsilon \cos \theta + \frac{[(2/3)\varepsilon - \mu B_0]}{\Omega_0^2} \frac{F^2}{f_0}.
$$
 (39)

This approximate result confirms the speculation made about the general case, namely that the contribution from the linear operator vanishes on the appropriate average, which in the banana regime is simply an unweighted θ average. Also, in the banana regime, the linear contribution is $\mathcal{O}(\epsilon)$ smaller than the nonlinear one.

Summary.—The implication is that if one attempts to improve upon standard neoclassical theory by retaining second- or higher-order poloidal ion gyroradius effects, a spurious solution will be obtained if the linearized collision operator is used. We have shown explicitly that in the banana regime the collisional contribution to the secondorder solution is correctly given only when $C(f_1, f_1)$ is retained. Indeed, new analytic gyrokinetic formulations already exist for which this term is included [[8\]](#page-3-8). Therefore, in general, nonlinear corrections to the collision operator must be accurately retained in full-f and hybrid fluid $\frac{1}{6}$ numerical simulations in order to avoid the type of spurious solution we have demonstrated in this Letter.

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