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J.B. Parker\* and P.J. Catto

\*Princeton University

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Plasma Science and Fusion Center Massachusetts Institute of Technology Cambridge MA 02139 USA

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## Variational Calculation of Neoclassical Ion Heat Flux in the Banana Regime for Axisymmetric Magnetic Geometry

J. B.  $Parker^1$  and P. J.  $Catto^2$ 

<sup>1</sup>Princeton University, Princeton, New Jersey 08544, USA <sup>2</sup>Plasma Science and Fusion Center, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

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#### Abstract

We present a numerical solution of the drift kinetic equation retaining the linearized Fokker-Planck collision operator which is valid for general axisymmetric magnetic geometry in the low collisionality limit. We use the well-known variational principle based on entropy production and expand in basis functions. Uniquely, we expand in pitch-angle basis functions which are eigenfunctions of the transit-averaged test particle collision operator. These eigenfunctions, which depend on the geometry, are extremely well suited to this problem, with only one or two basis functions required to obtain an accurate solution. As a simple example of the technique, the neoclassical ion heat flux and poloidal flow are calculated for circular flux surfaces and compared with analytic approximations for arbitrary aspect ratio.

#### I. INTRODUCTION

Neoclassical transport is concerned with the transport of particles, heat, momentum, and current due to collisional relaxation in an inhomogeneous magnetic geometry [1, 2]. Usually, neoclassical cross-field transport is overwhelmed by turbulent transport. However, under enhanced confinement conditions such as within an internal transport barrier, turbulence can be suppressed and ion thermal transport can be reduced to neoclassical levels [3]. As a result, there has been a revival of interest in accurate calculations of neoclassical transport.

Numerical solutions of the drift kinetic equation (DKE) have been carried out previously. The NEO code by Belli and Candy calculates neoclassical transport for arbitrary collisionality including multiple species [4]. In that work, collisions are incorporated through the Hirshman-Sigmar approximation [5] to the linearized Fokker-Planck collision operator. Recently, Wong and Chan have solved the first order DKE for a single ion species and arbitrary collisionality using the full linearized Fokker-Planck collision operator [6]. However, their technique converges too slowly in the limit of low collisionality and large aspect ratio to compare with the available exact results.

In this work we solve the first order ion DKE for a single ion species in the low collisionality limit using the full linearized Fokker-Planck operator. Our solution method uses a variational principle [7] for the first order DKE and is valid in arbitrary axisymmetric magnetic geometry. Uniquely, we use an expansion in pitch-angle basis functions which are eigenfunctions of the transit-averaged test particle collision operator [8–10]. These eigenfunctions, which depend on the geometry, turn out to be extremely well suited to this problem. Because we are considering weak collisionality, and not considering finite orbit width effects or coupling with electrons or impurities, our work should be viewed as a study of the importance of keeping the linearized Fokker-Planck collision operator without approximation. For concentric circular flux surfaces, we find that at intermediate aspect ratios, the well-known approximate analytic expressions accurately calculate the ion heat flux, but there are small corrections required for plasma flow. Our solution easily converges to the known results in the limit of large aspect ratio and unit aspect ratio.

#### **II. VARIATIONAL PRINCIPLE**

To examine the consequences of retaining the full linearized Fokker-Planck collision operator we work in the limit of small gyroradius and small normalized collisionality and retain a single ion species. The starting point for the theory is the drift-kinetic equation for the gyroaveraged ion distribution function f [1]. The primary ordering parameter is  $\delta \equiv \rho/L$ , where  $\rho = v_T/\Omega$  is the gyroradius, L is the macroscopic scale length,  $v_T = (2T/m)^{1/2}$  is the thermal speed,  $\Omega = ZeB/mc$  is the gyrofrequency, T is the ion temperature, Z and m are the ion charge number and mass, respectively, B is the magnetic field, and c is the speed of light. The equilibrium magnetic field is  $\mathbf{B} = \nabla \zeta \times \nabla \psi + I(\psi) \nabla \zeta$  where  $\zeta$  is the toroidal angle,  $\psi$  is the poloidal flux divided by  $2\pi$ ,  $I = RB_{\zeta}$ , and R is the major radius.

After expanding in small  $\delta$ , H-theorem arguments show that the lowest order distribution is Maxwellian on each flux surface,  $f_m = n/(\pi^{3/2}v_T^3) \exp(-v^2/v_T^2)$ , where n is the ion density [1]. The small  $\delta$  ordering implies behavior is local in  $\psi$ . Subsidiary expansion is performed in the limit of small normalized collisionality  $\nu_*$ , where  $\nu_* = \nu_{\text{eff}}/\omega_b$ ,  $\nu_{\text{eff}}$  is the effective scattering frequency of trapped particles, and  $\omega_b$  is the bounce frequency of trapped particles. One obtains the "collisional constraint equation" for the perturbed distribution function  $f_1$ [1, 7, 11]

$$\left\langle \frac{B}{v_{\parallel}}C(f_1) \right\rangle = 0, \tag{1}$$

where  $f = f_m + f_1$  and C is the linearized like-species Fokker-Planck collision operator. We neglect ion-electron collisions. The angle brackets denote a poloidal transit average, given by  $\langle y \rangle = \left( \oint d\theta \, y / \mathbf{B} \cdot \nabla \theta \right) / \int_0^{2\pi} d\theta / \mathbf{B} \cdot \nabla \theta$ , where  $\theta$  is the poloidal angle. The integral in the numerator goes from 0 to  $2\pi$  for untrapped particles and is a closed orbit between the turning points for trapped particles. We decompose  $f_1$  as

$$f_1 \equiv F + g, \tag{2}$$

where F is a known function and acts as a source term, and is given by

$$F = -\frac{Iv_{\parallel}}{\Omega} \left. \frac{\partial f_m}{\partial \psi} \right|_E = -\frac{Iv_{\parallel}}{\Omega} \left[ \frac{p'}{p} + \frac{q\Phi'}{T} + \left( \frac{v^2}{v_T^2} - \frac{5}{2} \right) \frac{T'}{T} \right] f_m. \tag{3}$$

Here the  $\psi$  derivative is taken at constant total energy  $E = mv^2/2 + Ze\Phi$ ,  $\Phi$  is the electric potential, p is the ion pressure and a prime denotes  $d/d\psi$ . The unknown function to be solved for is g, which depends only on constants of the motion and not on  $\theta$  [7]. The homogeneous solutions of Eq. (1) which may be added to g amount to a shift in the density or temperature of the full distribution function, so such homogeneous solutions are ignored. The integral in Eq. (1) annihilates the drive term F in the trapped region of phase space, and so g is zero in the trapped region. A consequence of the above is that g has a discontinuous derivative at the trapped-passing boundary. It has been shown that if one goes to next order in collisionality  $\nu_*$ , in actuality a boundary layer exists, and the discontinuity can be resolved [12].

A variational principle for the collisional constraint equation is given by the minimization of the entropy production integral [1, 7, 11]

$$S = -\left\langle \int d^3 v \frac{f_1}{f_m} C(f_1) \right\rangle.$$
(4)

To solve the collisional constraint equation, we can in principle evaluate Eq. (4) for many different trial functions  $f_1$  subject to the constraints. If the trial functions are chosen well, the  $f_1$  which gives the lowest value for S is closest to the true solution and presumably a good approximation. The constraints are Eq. (2) and the vanishing of g in the trapped region. Because the drive term is odd in  $v_{\parallel}$ , it is also clear that g will be odd in  $v_{\parallel}$ .

One way to parameterize the search space of all allowable functions g is to write g as an expansion in basis functions. For this purpose we use the velocity coordinates  $(v, \lambda, \sigma)$ , where  $\lambda \equiv v_{\perp}^2 \bar{B}/v^2 B$ ,  $\sigma \equiv \text{sign}(v_{\parallel})$ , and  $\bar{B}$  is the maximum magnetic field on a flux surface. We write g and  $f_1$  in the following normalized form:

$$g = Af_m \sum_i a_i B_i(x, \lambda, \sigma), \tag{5}$$

$$f_1 = A\left(\sum_i a_i B_i(x,\lambda,\sigma) - hx^3\xi\right) f_m - \frac{Iv_{\parallel}}{\Omega} \left[\frac{p'}{p} + \frac{q\Phi'}{T} - \frac{5}{2}\frac{T'}{T}\right] f_m,\tag{6}$$

where  $x \equiv v/v_T$  is the normalized speed,  $\xi = v_{\parallel}/v$ ,  $A \equiv Iv_T T'/\bar{\Omega}T$ ,  $\bar{\Omega} \equiv Ze\bar{B}/mc$ ,  $\kappa \equiv n/(\pi^{3/2}v_T^3)$  is defined through  $f_m = \kappa e^{-x^2}$ , and  $h(\theta) \equiv \bar{B}/B(\theta)$ . The basis functions  $B_i$  satisfy the same constraints as g, namely, they vanish in the trapped region and are odd in  $\sigma$ . The  $a_i$  are the unknown coefficients. Equation (4) becomes

$$\eta^{-1}S = -\left\langle \int d^3x \frac{f_1}{f_m} \frac{C(f_1)}{A^2 \kappa \nu_B} \right\rangle,\tag{7}$$

where  $\eta \equiv A^2 \pi^{-3/2} n \nu_B$  and  $\nu_B = 4\sqrt{\pi} Z^4 e^4 n \ln \Lambda_c / 3\sqrt{m} T^{3/2}$  is the Braginskii collision frequency. We substitute Eq. (6) into Eq. (7) and recognize that due to the conservation properties of the collision operator, the terms in square brackets in Eq. (6) are annihilated by the integral. We obtain

$$\eta^{-1}S = -\sum_{i,j} a_i a_j M_{ij} + 2\sum_i a_i b_i - \left\langle h^2 \int d^3 x \, x^3 \xi \widehat{C}_n\left(x^3 \xi\right) \right\rangle,\tag{8}$$

where  $\widehat{C}_n \equiv \widehat{C}/(\kappa\nu_B)$  is the normalized collision operator,  $\widehat{C}(\chi) \equiv C(\chi f_m)$ , and selfadjointness has been used. The matrix elements are given by

$$M_{ij} \equiv \left\langle \int d^3x \, B_i \widehat{C}_n(B_j) \right\rangle,\tag{9}$$

$$b_{i} \equiv \left\langle h \int d^{3}x \, B_{i} \widehat{C}_{n} \left( x^{3} \xi \right) \right\rangle = h \int d^{3}x \, B_{i} \widehat{C}_{n} \left( x^{3} \xi \right), \tag{10}$$

where M is a symmetric matrix as a result of self-adjointness. The second form of  $b_i$  without an explicit flux surface average holds because there is no  $\theta$  dependence left over when the velocity integral is done first. In matrix notation,

$$\eta^{-1}S = -a^T M a + 2a^T b + \eta^{-1}S_3, \tag{11}$$

where

$$\eta^{-1}S_3 \equiv -\left\langle h^2 \int d^3x \, x^3 \xi \widehat{C}_n\left(x^3\xi\right) \right\rangle = \pi^{3/2} \left\langle h^2 \right\rangle. \tag{12}$$

In evaluating Eq. (12) we used

$$d^{3}x = dx \, d\lambda \, d\varphi \sum_{\sigma} x^{2}/2h|\xi| \tag{13}$$

and

$$\frac{\widehat{C}_n(x^3\xi)}{\xi} = -\frac{30xe^{-2x^2} + 3e^{-x^2}\sqrt{\pi}(-5+2x^2)\operatorname{erf}(x)}{\sqrt{2}x^2},$$
(14)

the latter of which is independent of  $\xi$  due to the rotational symmetry of C.

We can minimize S in Eq. (8) with respect to each of the  $a_i$  by taking the partial derivative  $\partial/\partial a_i$  and setting it equal to 0, which yields a matrix equation for the coefficients  $a_j$ ,

$$Ma = b. (15)$$

While we have derived this matrix equation from the variational principle, it can also be derived directly from the collisional constraint equation. The same matrix equation is obtained from Eq. (1) by substituting in Eq. (6) and applying  $\sum_{\sigma} \sigma \int dv \, d\lambda \, v^2 B_j$ .

#### **III. BASIS FUNCTIONS**

We now turn to the question of exactly what basis function  $B_i(v, \lambda, \sigma)$  to use for our expansion. We let  $i \to \{l, n\}$  and use the separable form

$$B_{ln} = \sigma V_l(x) g_n(\lambda) \tag{16}$$

where l = 0, ..., L and n = 1, ..., N.

In the Spitzer problem, a Laguerre polynomial expansion is used and only the source terms  $b_0$  and  $b_1$  are nonzero; all the others vanish by orthogonality. This procedure leads to a rapid convergence of the coefficients as one increases the number of polynomials retained [11]. In the Spitzer problem, however, the source term was a polynomial in speed. In contrast, for our neoclassical problem the source term is  $\widehat{C}_N(x^3\xi)/\xi$  which is a complicated function of x involving error functions and exponentials in the definition. It is too much to hope that all the source terms are zero except for a finite number. However, it would be convenient if the source terms  $b_i$  decayed quickly as i increased. Then, perhaps the coefficients would converge rapidly. Then using Eqs. (16) and (14) in Eq. (10) gives

$$b_i \to b_{ln} = 2\pi \int_0^\infty dx \, x^2 V_l(x) \frac{\widehat{C}_n(x^3\xi)}{\xi} \int_0^{h_{\min}} d\lambda \, g_n(\lambda). \tag{17}$$

The two integrals in  $b_{ln}$ , x and  $\lambda$ , are independent. Ideally, the  $\lambda$  integral tends to zero for large n, while the speed integral tends to zero for large l. This behavior will be used as a criterion for determining appropriate basis functions for expansion. For convenience let

$$X_l \equiv \int_0^\infty dx \, x^2 V_l(x) \frac{\widehat{C}_n\left(x^3\xi\right)}{\xi},\tag{18}$$

$$\beta_n \equiv \int_0^{h_{\min}} d\lambda \, g_n(\lambda). \tag{19}$$

#### A. Basis function in x

For the speed basis functions a common choice is to involve the set of Laguerre polynomials  $L_l^{(3/2)}(x^2)$ . We use

$$V_l(x) = x L_l^{(3/2)} \left( x^2 \right).$$
(20)

A generating function for the generalized Laguerre polynomials is [13]

$$s(x,z;\alpha) = \frac{e^{-xz(1-z)}}{(1-z)^{\alpha+1}} = \sum_{l=0}^{\infty} L_l^{(\alpha)}(x)z^l,$$
(21)

which implies

$$L_l^{(\alpha)}(x) = \left. \frac{1}{l!} \frac{\partial^l s}{\partial z^l} \right|_{z=0}.$$
(22)

The generating function can be used to calculate the  $X_l$ . For  $\alpha = 3/2$ , we use Eq. (14) to find

$$q(z) \equiv \int_0^\infty dx \, x^3 s(x^2, z; 3/2) \frac{\widehat{C}_n(x^3\xi)}{\xi} = 3\sqrt{\frac{\pi}{2}} z(2-z)^{-3/2} \tag{23}$$

and

$$X_{l} = \frac{1}{l!} \frac{d^{l}q}{dz^{l}} \bigg|_{z=0} = \frac{3}{2^{l}} \frac{\Gamma(l+1/2)}{\Gamma(l)},$$
(24)

where  $\Gamma(x)$  is the gamma function. Observe that  $X_l$  decays as  $2^l$  for large l.

#### B. Basis function in $\lambda$

The primary requirement for the  $\lambda$  basis functions is that they are 0 in the trapped region. The passing region is given by  $0 < \lambda < 1$ , while the trapped region is given by  $1 < \lambda < h_{\text{max}}$ . We will use eigenfunctions of the transit-averaged test particle collision operator. The eigenfunctions are defined through a Sturm-Liouville problem as the solutions of [8–10]

$$\frac{d}{d\lambda}p(\lambda)\frac{dg_n}{d\lambda} + \mu_n w(\lambda)g_n = 0,$$
(25)

where

$$p(\lambda) \equiv \lambda \langle |\xi| \rangle, \tag{26}$$

$$w(\lambda) \equiv \left\langle \frac{1}{h|\xi|} \right\rangle,\tag{27}$$

with boundary conditions  $g(\lambda = 1) = 0$ , and at the lower boundary  $\lambda = 0$  we need only require that  $g_n$  and its derivative be finite. The  $\mu_n$  are the eigenvalues. This differential equation is a singular Sturm-Liouville problem with a complete set of orthogonal eigenfunctions satisfying the boundary conditions. We additionally normalize the eigenfunctions such that  $g_n(\lambda = 0) = 1$ .

The  $g_n$  must be found numerically by solving the Sturm-Liouville problem. We obtain a set of orthogonal eigenfunctions  $g_n(\lambda)$ , n = 1, 2, ... for which we define the following integrals:

$$M_n \delta_{nm} = \int_0^1 d\lambda \, w(\lambda) g_n(\lambda) g_m(\lambda), \qquad (28)$$

$$\beta_n = \int_0^1 d\lambda \, g_n(\lambda). \tag{29}$$

From the properties of Sturm-Liouville equations, each  $g_n$  has n zeroes. Therefore, as n increases the  $g_n$  become more oscillatory, so  $\beta_n$  tends to decrease to 0 for large n, as desired. In the  $\epsilon \to 0$  limit, the eigenfunctions are  $g_n(\lambda) = P_{2n-1}(\sqrt{1-\lambda})$  with eigenvalues  $\mu_n = 2n(2n-1)/4$ ,  $\beta_n = 2\delta_{n1}/3$  and  $M_n = 2/(4n-1)$ , where the  $P_n$  are the Legendre polynomials [10].

These pitch-angle eigenfunctions have the advantage that they depend on the magnetic geometry, which removes the explicit geometric dependence from other parts of the calculation. In particular, the integrals involving the test part of the collision operator can be performed easily. In addition, in the large aspect ratio limit, the  $g_1$  term dominates in an  $\epsilon^{1/2}$  expansion, making the large aspect ratio limit easy to solve.

Figure 1 shows the first few eigenfunctions for the circular flux surface geometry described in Eq. (30) with  $\epsilon = 0.3$ . The first eigenfunction  $g_1(\lambda)$  (blue solid line) can be compared with the  $\lambda$  dependence obtained when solving the collisional constraint equation with only the pitch-angle scattering collision operator. In that case the lambda dependence is given by the solution of the differential equation (pg')' = constant, or  $g_R(\lambda) = N_0 \int_{\lambda}^1 d\lambda' / \langle \sqrt{1 - \lambda'/h} \rangle$ (blue dashed line), where  $N_0$  is a normalization constant. The two functions  $g_1(\lambda)$  and  $g_R(\lambda)$ are fairly close, and it can be shown they differ by  $O(\epsilon^{1/2})$  in the large aspect ratio limit.

#### IV. SOLVING THE MATRIX EQUATION

#### A. Model Magnetic Field

The technique as described is valid for arbitrary magnetic geometry. However, to compare with previous results, and as a particular example, we next consider a model magnetic field with concentric circular flux surfaces.

$$\mathbf{B} = \frac{\bar{B}(1-\epsilon)}{1+\epsilon\cos\theta} \frac{\hat{\varphi}+k\hat{\theta}}{\sqrt{1+k^2}},\tag{30}$$



FIG. 1. Pitch-angle eigenfunctions (solid lines)  $g_n(\lambda)$  for n = 1, ..., 5, using the circular flux surface geometry with  $\epsilon = 0.3$ . The first eigenfunction  $g_1(\lambda)$  is close to  $g_R(\lambda)$  (dashed line), the pitch-angle dependence obtained when the collisional constraint equation is solved retaining only the pitch-angle scattering operator.

where k is only a function of radius. Then

$$h(\theta) = \frac{1 + \epsilon \cos \theta}{1 - \epsilon} \tag{31}$$

and the flux surface average of a quantity y is given by

$$\langle y \rangle = \frac{1}{2\pi} \int_0^{2\pi} d\theta \, y (1 + \epsilon \cos \theta). \tag{32}$$

#### **B.** Matrix Elements

The computation of the source terms  $b_i$  has been described already in Section III. We now describe the procedure to compute the matrix elements  $M_{ij}$  in Eq. (9). We begin by decomposing the collision operator into the pitch-angle scattering, energy diffusion, and field terms.

$$\widehat{C}_n \equiv \widehat{C}_n^p + \widehat{C}_n^E + \widehat{C}_n^{Fa} + \widehat{C}_n^{Fb}, \qquad (33)$$

where

$$\widehat{C}_{n}^{p}(\chi) = e^{-x^{2}} |\xi| h \bar{\nu}_{\perp} \frac{\partial}{\partial \lambda} \lambda |\xi| \frac{\partial \chi}{\partial \lambda}, \qquad (34)$$

$$\widehat{C}_{n}^{E}(\chi) = \frac{1}{2x^{2}} \frac{\partial}{\partial x} e^{-x^{2}} x^{4} \bar{\nu}_{\parallel} \frac{\partial \chi}{\partial x}, \qquad (35)$$

$$\widehat{C}_n^{Fb}(\chi) = 3\sqrt{2}e^{-2x^2}\chi.$$
(36)

The remaining part of the field operator  $\widehat{C}_n^{Fa}$  is more complicated and is given shortly. Here  $\bar{\nu}_{\perp}(x) \equiv \nu_{\perp}(x)/\nu_B$ ,  $\bar{\nu}_{\parallel}(x) \equiv \nu_{\parallel}(x)/\nu_B$ ,  $\nu_{\perp}(x) = \nu_B 3\sqrt{2\pi} [\operatorname{erf}(x) - \Psi(x)]/2x^3$ ,  $\nu_{\parallel}(x) = \nu_B 3\sqrt{2\pi}\Psi(x)/2x^3$ ,  $\operatorname{erf}(x)$  is the error function, and  $\Psi(x) = [\operatorname{erf}(x) - x \operatorname{erf}'(x)]/2x^2$  is the Chandrasekhar function. The matrix elements involving  $\widehat{C}_n^p$ ,  $\widehat{C}_n^E$ , and  $\widehat{C}_n^{Fb}$  can be calculated analytically. Decomposing the  $M_{ij}$  as in Eq. (33) and using Eqs. (16), (20), and (34)–(36) in (9), we obtain after some algebra

$$M_{ij}^{p} = (-\mu_{n} K_{ll'}^{p}) \, 2\pi \delta_{nn'} M_{n}, \tag{37}$$

$$M_{ij}^E = \left(K_{ll'}^E/2\right) 2\pi \delta_{nn'} M_n,\tag{38}$$

$$M_{ij}^{Fb} = \left(3\sqrt{2}K_{ll'}^{Fb}\right)2\pi\delta_{nn'}M_n,\tag{39}$$

where

$$K_{ll'}^{p} \equiv \int_{0}^{\infty} dx \, e^{-x^{2}} x^{4} \bar{\nu}_{\perp} L_{l}^{(3/2)} \left(x^{2}\right) L_{l'}^{(3/2)} \left(x^{2}\right), \tag{40}$$

$$K_{ll'}^E \equiv \int_0^\infty dx \, x L_l^{(3/2)} \left(x^2\right) \frac{d}{dx} e^{-x^2} x^4 \bar{\nu}_{\parallel} \frac{d}{dx} \left[x L_{l'}^{(3/2)} \left(x^2\right)\right],\tag{41}$$

$$K_{ll'}^{Fb} \equiv \int_0^\infty dx \, e^{-2x^2} x^4 L_l^{(3/2)} \left(x^2\right) L_{l'}^{(3/2)} \left(x^2\right). \tag{42}$$

An integration by parts could be applied to Eq. (41) to make the integral manifestly symmetric in l and l'. The speed integrals can be computed directly. Alternatively, the generating function technique used in Section III A can simplify the calculations somewhat. It is difficult to find closed-form expressions for  $K_{ll'}^p$  and  $K_{ll'}^E$ , but it is relatively straightforward to use the generating function to find

$$K_{ll'}^{Fb} = \frac{1}{2^{7/2}} \frac{\Gamma(l+l'+5/2)}{l!\,l'!\,2^{l+l'}}.$$
(43)

The contribution to  $M_{ij}$  from the final piece of the collision operator,  $\widehat{C}_n^{Fa}$ , must be calculated numerically.  $\widehat{C}_n^{Fa}$  is given by [14]

$$\widehat{C}_{n}^{Fa}\chi = \frac{3}{\pi\sqrt{8}}e^{-x^{2}} \left[\frac{2v^{2}}{v_{T}^{4}}\frac{\partial^{2}G_{1}}{\partial v^{2}} - \frac{2}{v_{T}^{2}}H_{1}\right],$$
(44)

where the Rosenbluth potentials are

$$G_1 = \int d^3v' f_m(v')\chi(\mathbf{v}')u, \qquad (45)$$

$$H_1 = \int d^3 v' f_m(v') \chi(\mathbf{v}') u^{-1}, \qquad (46)$$

$$u = |\mathbf{v} - \mathbf{v}'|. \tag{47}$$

In normalized variables with  $\mathbf{y} = \mathbf{v}'/v_T$ , this becomes

$$\widehat{C}_{n}^{Fa}(\chi) = \frac{3}{\pi\sqrt{8}} e^{-x^{2}} \int d^{3}y \, e^{-y^{2}} \chi(\mathbf{y}) U(u), \tag{48}$$

where now  $u = |\mathbf{x} - \mathbf{y}|$  and

$$U(u) \equiv 2x^2 \frac{\partial^2 u}{\partial x^2} - \frac{2}{u} \tag{49}$$

$$=\frac{x^2+y^2-2}{u}-\frac{u}{2}-\frac{(x^2-y^2)^2}{2u^3}.$$
(50)

Substituting into Eq. (9) gives

$$M_{ij}^{Fa} = \frac{3}{\pi\sqrt{8}} \left\langle \int d^3x \, d^3y \, \sigma_x \sigma_y e^{-(x^2 + y^2)} g_n(\lambda_x) g_{n'}(\lambda_y) V_l(x) V_{l'}(y) U(u) \right\rangle.$$
(51)

This expression is symmetric in swapping (l, l') or (n, n') independently. That is, we not only have  $M_{lnl'n'} = M_{l'n'ln}$  from self adjointness, but we also have  $M_{lnl'n'} = M_{ln'l'n}$ .

In the Appendix, we simplify Eq. (51) into a form appropriate for numerical integration.

#### C. Calculation of Neoclassical Quantities

Once the matrix coefficients  $M_{ij}$  have been calculated, Eq. (15) can be solved for the coefficients  $a_i$ . With the  $a_i$  known, the distribution function  $f_1$  is given by Eqs. (2) and (3) or equivalently by Eq. (6), and the neoclassical quantities of interest can be computed. We demonstrate the calculations of ion heat flux and plasma flow. We can relate S to the heat flux through

$$S = -\frac{1}{T^2} \frac{dT}{d\psi} \left\langle \mathbf{q} \cdot \nabla \psi \right\rangle.$$
(52)

After some manipulation, this yields

$$\left(\frac{nI^2}{m\bar{\Omega}^2}TT'\nu_B\right)^{-1}\langle \mathbf{q}\cdot\nabla\psi\rangle = -\frac{2}{\pi^{3/2}}\left(-a^TMa + 2a^Tb + \pi^{3/2}\langle h^2\rangle\right)$$
(53)

$$= -\frac{2}{\pi^{3/2}} \left( a^T b + \pi^{3/2} \langle h^2 \rangle \right).$$
 (54)

The second line would have been obtained if we used the collisional moment expression for heat flux directly.

The poloidal flow is calculated from [11]

$$n_i v_{i\theta} = K(\psi) B_{\theta},\tag{55}$$

where

$$K(\psi) \equiv \frac{1}{B} \int d^3 v \, v_{\parallel} g. \tag{56}$$

We obtain

$$\left(\frac{nIT'}{m\bar{\Omega}\bar{B}}\right)^{-1}K = \frac{3}{2}\sum_{n}a_{0n}\beta_{n}.$$
(57)

The parallel flow is given by

$$n_i v_{i\parallel} = \int d^3 v \, v_{\parallel} f_1 = -\frac{I}{m\Omega} \left( \frac{dp}{d\psi} + Zen \frac{d\Phi}{d\psi} \right) + \frac{KB}{n}.$$
(58)

#### D. Previous Approximate Analytic Results

For later use in comparing with our results, we quote some previous analytic results which have been obtained approximately. The Chang-Hinton formula for ion heat flux is an interpolation between large aspect ratio and unit aspect ratio using a single approximate result at intermediate aspect ratio. Simplified to circular flux surface geometry it is [15]

$$\alpha_q^{-1} \langle \mathbf{q} \cdot \nabla \psi \rangle = 2\epsilon^{1/2} \left( 0.66 + 1.88\epsilon^{1/2} - 1.54\epsilon \right) \left( 1 + 3\epsilon^2/2 \right), \tag{59}$$

where  $\alpha_q \equiv (nI^2TT'\nu_B/m\Omega_0^2)$ , and  $\Omega_0 \equiv ZeB_0/mc$  uses the magnetic field at  $\theta = \pi/2$ . The two field strengths  $B_0$  and  $\bar{B}$  are related by  $\bar{B} = B_0h(\pi/2)$ .

Taguchi's method involves assuming a particular form for the pitch-angle dependence of gand expanding the speed dependence in Laguerre polynomials. The pitch-angle dependence is assumed to be the  $g_R(\lambda)$  shown in Figure 1. The Taguchi formulas for ion heat flux and poloidal flow keeping 2 Laguerre polynomials are [11, 16]

$$\alpha_q^{-1} \langle \mathbf{q} \cdot \nabla \psi \rangle = 2 \left( \frac{\langle h^2 \rangle}{h(\pi/2)^2} - \frac{B_0^2}{\langle B^2 \rangle} \frac{f_c}{f_c + 0.462 f_t} \right), \tag{60}$$

$$\alpha_K^{-1} K = \frac{B_0^2}{\langle B^2 \rangle} \frac{1.17 f_c}{f_c + 0.462 f_t},\tag{61}$$

where  $\alpha_K \equiv (nIT'/m\Omega_0B_0)$ ,

$$f_t \equiv 1 - \frac{3}{4} \int_0^{h_{\min}^h} \frac{\lambda \, d\lambda}{\langle \sqrt{1 - \lambda/h^h} \rangle},\tag{62}$$

 $h^h(\theta) \equiv \langle B^2 \rangle^{1/2} / B$ , and  $f_c \equiv 1 - f_t$ . For the model magnetic field,  $\langle B^2 \rangle^{1/2} = B_0 (1 - \epsilon^2)^{-1/4}$ and  $h^h = (1 - \epsilon)(1 - \epsilon^2)^{-1/4} h$ .



FIG. 2. Convergence of the (a) heat flux and (b) poloidal flow at  $\epsilon = 0.3$  as a function of the number of pitch-angle eigenfunctions kept, N. Here we use L = N, i.e. one more Laguerre polynomial than pitch-angle eigenfunction.

#### V. RESULTS

We present the results of the numerical solution using the model magnetic field with circular flux surfaces. First we show the convergence results vs. the number of pitch-angle eigenfunctions kept, N, using  $\epsilon = 0.3$ . For these results, the number of Laguerre polynomials kept is N + 1, i.e. L = N. The results are presented in Figure 2. To get within 1% and 0.1% of the N = 6 solution (taken to be correct) requires N = 2 and N = 5 respectively. As required by the variational nature of the problem, the heat flux decreases monotonically as N is increased. The behavior is similar at other  $\epsilon$ .

We show the heat flux and poloidal flow for several values of  $\epsilon$  computed with N = 1and N = 2 (again L = N). In Figure 3(a) the heat flux is compared with the formulas of Chang-Hinton and Taguchi (we normalize our formulas to use  $B_0$  instead of  $\overline{B}$ ). Those approximate analytical formulas are in good agreement with our exact solution even at finite aspect ratio. In Figure 3(b) our poloidal flow is compared with the analytic formula derived using Taguchi's method [11]. The analytic formula does reasonably well but can have errors of up to 20% at intermediate aspect ratios. We also observe that our poloidal flow value  $\alpha_K^{-1}K$  agrees with Figure 8 of Ref. [6] when those results at finite aspect ratio are extrapolated to zero collisionality.

We have fit our heat flux and poloidal flow curves to polynomials in  $\epsilon^{1/2}$  which interpolate



FIG. 3. (a) Heat flux and (b) poloidal flow at several values of  $\epsilon$ , using N = 1 and N = 2. Here we use L = N, i.e. one more Laguerre polynomial than pitch-angle eigenfunction. The exact numerical solutions are compared with the Chang-Hinton and Taguchi formulas.

over finite aspect ratios. It is quite adequate to include four terms in each:

$$\alpha_q^{-1} \langle \mathbf{q} \cdot \nabla \psi \rangle = 1.34 \epsilon^{1/2} + 2.60 \epsilon - 2.13 \epsilon^{3/2} + 3.18 \epsilon^2, \tag{63}$$

$$\alpha_K^{-1}K = 1.17 - 1.22\epsilon^{1/2} - 0.68\epsilon + 0.72\epsilon^{3/2}.$$
(64)

#### VI. SUMMARY

We have developed a method for evaluating neoclassical transport in the core of a tokamak with general magnetic geometry in the low collisionality limit. We have demonstrated that analytic methods which approximate the collision operator are accurate at intermediate aspect ratios for estimating the ion heat flux but can be off by up to 20% at intermediate aspect ratios for estimating the poloidal flow. While we have used circular flux surfaces here, it is straightforward to apply the method to more general geometry. Multiple species could in principle be used as well.

The variational principle we use only applies in the limit of small collisionality and orbit width. When these restrictions are lifted, our technique cannot be used directly in those more general situations where finite collisionality or finite orbit width effects are retained. These important cases must be studied using other means. However, our work efficiently describes the effects of retaining the exact linearized Fokker-Planck collision operator as opposed to common approximations to the collision operator to make the calculations more analytically tractable.

The effectiveness of our calculation is a direct result of using the pitch-angle eigenfunctions associated with the transit-averaged test particle collision operator. These eigenfunctions, which depend on the magnetic geometry, are extremely well suited to this problem, with only one or two basis functions required to obtain an accurate solution.

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# Appendices

### Appendix A: Evaluation of $M_{ij}^{Fa}$

We simplify Eq. (51) into a form suitable for numerical integration. The integral is written in coordinates using Eq. (13). The gyrophase integral over  $\varphi_y$  can be done analytically [14]:

$$I \equiv \int_{0}^{2\pi} d\varphi_y U(u) = \frac{4(x^2 + y^2 - 2)}{\Lambda} K(\kappa) - 2\Lambda E(\kappa) - \frac{2(x^2 - y^2)^2}{\Lambda^3} \frac{E(\kappa)}{1 - \kappa^2},$$
 (A1)

where here K and E are the complete elliptic integrals of the first and second kind with the modulus as argument, and

$$\Lambda^2 \equiv x^2 + y^2 + 2x_{\perp}y_{\perp} - 2x_{\parallel}y_{\parallel}, \tag{A2}$$

$$\kappa^2 \equiv \frac{4x_\perp y_\perp}{\Lambda^2},\tag{A3}$$

 $x_{\parallel} \equiv \sigma_x x \sqrt{1 - \lambda_x/h}, \ \sigma_x \equiv \operatorname{sign}(x_{\parallel}), \ x_{\perp} \equiv x \sqrt{\lambda_x/h}, \ \text{and similarly for } y_{\parallel} \ \text{and } y_{\perp}.$  Then let

$$\sum_{\sigma_y} \sigma_y I = \sigma_x I_1(x, \lambda_x, y, \lambda_y, \theta), \tag{A4}$$

where  $I_1 \equiv I(\sigma_x = +1, \sigma_y = +1) - I(\sigma_x = +1, \sigma_y = -1)$ . We have pulled out a factor of  $\sigma_x$ and evaluated at  $\sigma_x = +1$  because the expression is odd in  $\sigma_x$ . Explicitly,

$$I_{1} = 4(x^{2} + y^{2} - 2) \left[ \frac{K_{+}}{\Lambda_{+}} - \frac{K_{-}}{\Lambda_{-}} \right] - 2 \left[ \Lambda_{+} E_{+} - \Lambda_{-} E_{-} \right] - 2(x^{2} - y^{2})^{2} \left[ \frac{E_{+}}{\Lambda_{+}^{3}(1 - \kappa_{+}^{2})} - \frac{E_{-}}{\Lambda_{-}^{3}(1 - \kappa_{-}^{2})} \right],$$
(A5)

where

$$\Lambda_{\pm}^{2} \equiv \Lambda^{2}(\sigma_{x} = \pm 1, \sigma_{y} = \pm 1) = x^{2} + y^{2} + 2xy \left[\sqrt{\frac{\lambda_{x}\lambda_{y}}{h^{2}}} \mp \sqrt{\left(1 - \frac{\lambda_{x}}{h}\right)\left(1 - \frac{\lambda_{y}}{h}\right)}\right], \quad (A6)$$

$$\kappa_{\pm}^2 \equiv \frac{4xy\sqrt{\lambda_x\lambda_y}}{h\Lambda_{\pm}^2},\tag{A7}$$

$$K_{\pm} \equiv K(\kappa_{\pm}),\tag{A8}$$

$$E_{\pm} \equiv E(\kappa_{\pm}). \tag{A9}$$

The  $\sigma_x$  sum may be performed to gain a factor of 2. Equation (51) becomes

$$M_{ij}^{Fa} = \frac{3}{\sqrt{8}} \left\langle \frac{1}{h^2} \int d\lambda_x \, d\lambda_y \, \frac{g_n(\lambda_x)g_{n'}(\lambda_y)}{|\xi_x||\xi_y|} A_{ll'} \right\rangle,\tag{A10}$$

with

$$A_{ll'}(\lambda_x, \lambda_y, \theta) \equiv \int_0^\infty \int_0^\infty dx \, dy \, e^{-(x^2 + y^2)} x^3 y^3 L_l^{(3/2)}(x^2) L_{l'}^{(3/2)}(y^2) I_1.$$
(A11)

One more integral may be performed analytically by converting to polar coordinates,  $x = r \cos \phi$ ,  $y = r \sin \phi$ . Then

$$\int_{0}^{\infty} dx \, \int_{0}^{\infty} dy = \int_{0}^{\pi/2} d\phi \int_{0}^{\infty} dr \, r.$$
 (A12)

Importantly,  $\kappa_{\pm}$  does not depend on r and the r integral is elementary. After some algebra, we have

$$A_{ll'} = \int_0^{\pi/2} d\phi \, \sin^3 2\phi \left[ cC_{ll'} + dD_{ll'} \right], \tag{A13}$$

where

$$C_{ll'} \equiv \frac{1}{2^3} \int_0^\infty dr \, e^{-r^2} r^6 \left[ 4 \left( r^2 - 2 \right) \right] L_l^{(3/2)} \left( r^2 \cos^2 \phi \right) L_{l'}^{(3/2)} \left( r^2 \sin^2 \phi \right), \tag{A14}$$

$$D_{ll'} \equiv \frac{1}{2^3} \int_0^\infty dr \, e^{-r^2} r^6 \left(-2r^2\right) L_l^{(3/2)} \left(r^2 \cos^2 \phi\right) L_{l'}^{(3/2)} \left(r^2 \sin^2 \phi\right),\tag{A15}$$

$$c \equiv \frac{K_{+}}{L_{+}} - \frac{K_{-}}{L_{-}},\tag{A16}$$

$$d \equiv (L_{+}E_{+} - L_{-}E_{-}) + \cos^{2}2\phi \left[\frac{E_{+}}{L_{+}^{3}(1 - \kappa_{+}^{2})} - \frac{E_{-}}{L_{-}^{3}(1 - \kappa_{-}^{2})}\right],$$
 (A17)

$$L_{\pm}^{2} \equiv \Lambda_{\pm}^{2}/r^{2} = 1 + \sin^{2}2\phi \left[\sqrt{\frac{\lambda_{x}\lambda_{y}}{h^{2}}} \mp \sqrt{\left(1 - \frac{\lambda_{x}}{h}\right)\left(1 - \frac{\lambda_{y}}{h}\right)}\right],$$
 (A18)

$$\kappa_{\pm}^2 = \frac{2\sqrt{\lambda_x \lambda_y} \sin 2\phi}{hL_{\pm}^2}.$$
(A19)

After putting the  $\theta$  integral in explicitly, we finally have

$$M_{ij}^{Fa} = \frac{3}{\sqrt{8}} \int d\lambda_x \, d\lambda_y \, g_n(\lambda_x) g_{n'}(\lambda_y) \gamma_{ll'}(\lambda_x, \lambda_y), \tag{A20}$$

where

$$\gamma_{ll'}(\lambda_x,\lambda_y) \equiv \left(\int_0^{2\pi} \frac{d\theta}{\mathbf{B}\cdot\nabla\theta}\right)^{-1} \int_0^{2\pi} d\theta \int_0^{\pi/2} d\phi \,\frac{\sin^3 2\phi \left[cC_{ll'} + dD_{ll'}\right]}{h^2(\mathbf{B}\cdot\nabla\theta)|\xi_x||\xi_y|}.$$
(A21)

This form is used for numerical integration. The four-dimensional integration is performed using the NAG C Library. The  $\theta$  and  $\phi$  integrals are computed using two-dimensional adaptive quadrature on a discrete  $(\lambda_x, \lambda_y)$  grid to give  $\gamma_{ll'}$ . The eigenfunctions  $g_n$  are computed on this grid, and a discrete integration method is used to perform the two  $\lambda$  integrals.

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