

## Computation of neoclassical transport in stellarators using the full linearized Coulomb collision operator \*

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Fast and accurate computations of transport coefficients, bootstrap current and the generalized Spitzer function in stellarators is an important problem for stellarator optimization, generation of neoclassical data bases, and modelling of the current drive. In this report a new field line integration method for these purposes is presented. For the computation, the distribution function  $f$  can be linearized,  $f = f_0(\psi, v) + \delta f(\psi, s, v, \lambda)$ , and expanded over energy as follows,

$$\begin{aligned} \delta f(\psi, s, v, \lambda) &= f_0(\psi, v) \sum_m f_m(\psi, s, \lambda) \varphi_m(v/v_T), \\ \varphi_m(x) &= \pi^{3/4} \sqrt{\frac{2\Gamma(m+1)}{\Gamma(m+5/2)}} L_m^{(3/2)}(x^2), \end{aligned} \quad (1)$$

where  $L_m^{(n)}$  are Laguerre polynomials. In regimes with small poloidal drift, the linearized drift kinetic equation (DKE) can be written as,

$$\sigma \frac{\partial f_m^\sigma}{\partial s} - \kappa \sum_{m'} \left\{ v_{mm'} \mathcal{L} f_{m'}^\sigma + \mathcal{K}_{mm'} f_{m'}^\sigma + \frac{1}{|\lambda|} D_{mm'} f_{m'}^\sigma \right\} = -\frac{v_T}{\omega_c} \left( A_1 a_m^{(1)} + A_2 a_m^{(2)} \right) q_G^\sigma - A_3 a_m^{(3)} q_E^\sigma \quad (2)$$

with the pitch-angle scattering operator

$$\mathcal{L} f_{m'}^\sigma = \frac{1}{4|\lambda|} \frac{\partial}{\partial \lambda} (1 - \lambda^2) \frac{\partial}{\partial \lambda} f_{m'}^\sigma(\psi, s, \lambda) = \frac{\partial}{\partial \eta} \left( \frac{\eta|\lambda|}{\hat{B}} \right) \frac{\partial}{\partial \eta} f_{m'}^\sigma(\psi, s, \eta), \quad (3)$$

and the integral part of the linearized collision operator

$$\mathcal{K}_{mm'} f_{m'}^\sigma = \frac{1}{|\lambda|} \sum_\ell I_{mm'}^\ell P_\ell(\lambda) \int_{-1}^1 d\lambda' P_\ell(\lambda') f_{mm'}^{\sigma'}(\psi, s, \lambda'), \quad (4)$$

where for the expansion over  $\lambda$  the Legendre polynomials  $P_\ell$  are used. Here,  $\psi$  is a flux surface label,  $s$  is the distance counted along the m.f.l.,  $\lambda = v_{||}/v$  is pitch,  $\sigma$  is a sign of  $v_{||}$ ,  $\eta = (1 -$

\*This work has been carried out within the Association EURATOM-ÖAW and with funding from the Austrian Science Fund (FWF) under contract P16797-N08.

$\lambda^2)/\hat{B}$  is a normalized perpendicular invariant (magnetic moment),  $\hat{B} = B/B_0$  is the magnetic field module normalized to some reference magnetic field  $B_0$ ,  $\kappa = 4/l_c$  with  $l_c$  being the mean free path,  $v_T$  and  $\omega_c$  are thermal velocity and cyclotron frequency, respectively. The quantities  $v_{mm'}$ ,  $I_{mm'}$ ,  $D_{mm'}$  and  $a_m^{(i)}$  are matrix elements independent of plasma parameters, whereas the quantities  $A_i$  are the driving forces defined as,

$$A_1 = \frac{1}{n} \frac{\partial n}{\partial \psi} - \frac{3}{2T} \frac{\partial T}{\partial \psi} + \frac{e}{T} \frac{\partial \Phi}{\partial \psi}, \quad A_2 = \frac{1}{T} \frac{\partial T}{\partial \psi}, \quad A_3 = -\frac{e}{T} \frac{\langle E_{\parallel} \hat{B} \rangle}{\langle \hat{B}^2 \rangle}. \quad (5)$$

The source terms  $q_I^{\sigma}$  with drives  $I = G, E$  by gradient and by parallel electric field, respectively, are defined as

$$q_G^{\sigma} = \frac{\partial}{\partial \eta} \left( \frac{|\lambda|}{\hat{B}} \hat{V}_G \right), \quad q_E^{\sigma} = \sigma \hat{B}, \quad \hat{V}_G = \frac{1}{3} \left( \frac{4}{\hat{B}} - \eta \right) |\nabla \psi| k_G, \quad (6)$$

and  $k_G$  being the geodesic curvature. As a result of computations one obtains radial particle and heat flux densities and the bootstrap current as,

$$\begin{aligned} F_n &= \frac{nv_T^2}{\omega_c} \frac{1}{\langle |\nabla \psi| \rangle} \sum_m \sum_{\sigma} b_m^{(1)} \left\langle \hat{B} \int_0^{1/\hat{B}} d\eta f_m^{\sigma} q_G^{-\sigma} \right\rangle, \\ F_w &= \frac{nTv_T^2}{\omega_c} \frac{1}{\langle |\nabla \psi| \rangle} \sum_m \sum_{\sigma} b_m^{(2)} \left\langle \hat{B} \int_0^{1/\hat{B}} d\eta f_m^{\sigma} q_G^{-\sigma} \right\rangle, \\ \frac{\langle j_{\parallel} B \rangle}{\langle B^2 \rangle} &= \frac{nev_T}{B_0} \frac{1}{\langle \hat{B}^2 \rangle} \sum_m \sum_{\sigma} b_m^{(3)} \left\langle \hat{B} \int_0^{1/\hat{B}} d\eta f_m^{\sigma} q_E^{-\sigma} \right\rangle, \end{aligned} \quad (7)$$

where  $b_m^{(i)}$  are, again, numerical coefficients independent of problem parameters. All quantities  $\langle \dots \rangle$  are flux surface averages which are computed as field line averages using

$$\frac{\langle \alpha \rangle}{\langle \beta \rangle} = \lim_{L \rightarrow \infty} \int_0^L \frac{ds}{B} \alpha / \int_0^L \frac{ds}{B} \beta. \quad (8)$$

Putting the driving forces  $A_2 = A_3 = 0$ , one can compute normalized diffusion and bootstrap coefficients,

$$\frac{D_{11}}{D_{\text{plateau}}} = -\frac{F_n}{nA_1 \langle |\nabla \psi| \rangle D_{\text{plateau}}}, \quad \lambda_{bb} = -\frac{\langle j_{\parallel} B \rangle}{nA_1 T c \langle |\nabla \psi| \rangle}, \quad (9)$$

respectively. To regain the Lorentz model, one has to put  $m = m' = 0$ ,  $v_{00} = 1$  and  $D_{mm'} = I_{mm'}^{\ell} = 0$ ,  $a_0^{(1)} = 1$ ,  $b_0^{(1)} = 1/4$  and  $b_0^{(3)} = 3/8$ .

The set of coupled equations (2) is used by the field line tracing code NEO-2 introduced in [1] for the Lorentz collision model. For this purpose, equations (2) are discretized on an adaptive grid of  $\eta$ -values and the resulting set of coupled ordinary differential equations is solved. For benchmarking purposes, also a Monte Carlo technique, which belongs to the group

of  $\delta f$ -methods [2], is used. The Monte Carlo method itself is restricted to the use of the Lorentz collision model. Within this method, the solution of the linearized DKE, which can be formally written as

$$\frac{\partial \delta f}{\partial t} + V^i \frac{\partial \delta f}{\partial z^i} - \mathcal{L}_C \delta f = Q, \quad (10)$$

where  $\mathbf{z}$  is a set of phase space variables  $z^i$ ,  $V^i$  is a phase space drift motion velocity,  $\mathcal{L}_C$  is a Lorentz collision operator and  $Q$  is a source term, is approximated by the following expectation value

$$\delta f(\mathbf{z}) = \frac{1}{J(\mathbf{z})} \lim_{K \rightarrow \infty} \overline{\sum_{k=0}^K w \delta(\mathbf{z} - \mathbf{z}_k)}, \quad \overline{w \delta(\mathbf{z} - \mathbf{z}_0)} = J(\mathbf{z}) Q(\mathbf{z}) \Delta t. \quad (11)$$

Here  $\mathbf{z}_k$  are positions of a test particle after  $k$  integration steps of the stochastic orbit,  $J(\mathbf{z})$  is a phase space Jacobian,  $\Delta t$  is an integration time step and  $w$  is a test particle weight. Last equation (11) defines  $w$  via the source term. Note that contribution of large  $k$  to the infinite sum in (11) becomes exponentially small due to the relaxation by collisions and parallel motion, and, therefore, the stochastic orbits need to be followed only few collision times. For the reduction of variance, the method of antithetic variates has been used. Namely, taking the starting points  $\mathbf{z}_0$  evenly distributed over the flux surface and pitch  $\lambda$  one can use the symmetry of the source term (6) over  $\lambda$ . For this, a pair of particles with equal weights and opposite  $\lambda$  values is always generated and the same series of random numbers is used for both test particles when modelling the pitch angle scattering.

In Figs. 1 and 2 the result of computations of the perturbed distribution function by NEO-2 is shown for a relatively low collisionality case. One can see that this distribution function in a stellarator is rapidly varying with pitch which usually causes convergence problems in DKE solvers. In Figs. 3 and 4 the results of NEO-2 for a tokamak case are compared with the Monte Carlo method (red markers) and the asymptotical long mean free path theory (black). Green curves show the results of NEO-2 for the full collision operator and blue curves for the Lorentz model. One can see that this theory gives a good estimate of the bootstrap current in a relatively wide range of collisionalities. This is also the case for the normalized diffusion coefficient in stellarators (Fig. 5). In stellarators, typically, the computation of the bootstrap coefficient is more complicated and the asymptotic value is only reached at extremely low collisionalities (Fig. 6).

## References

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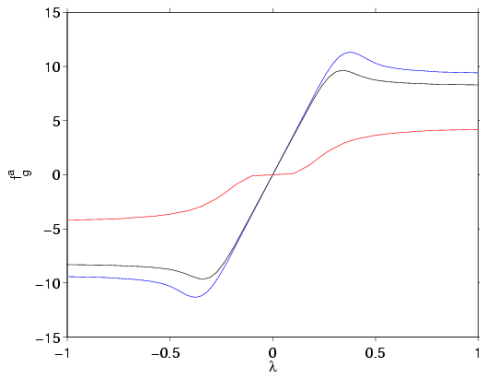


Fig. 1: Asymmetric part of the distribution function (gradient drive) for a Tokamak with  $2\pi R/l_c = 2 \cdot 10^{-3}$  at different poloidal positions (red: high field; black: top; blue: low field).

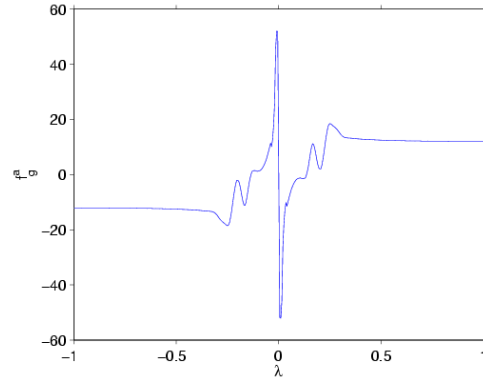


Fig. 2: Asymmetric part of the distribution function (gradient drive) for W7-AS with  $2\pi R/l_c = 1 \cdot 10^{-4}$ .

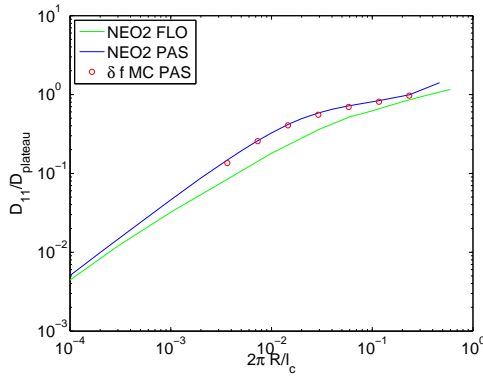


Fig. 3: Normalized diffusion coefficient for a Tokamak.

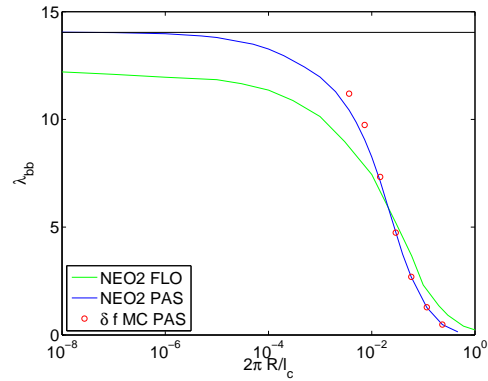


Fig. 4: Bootstrap coefficient for a Tokamak.

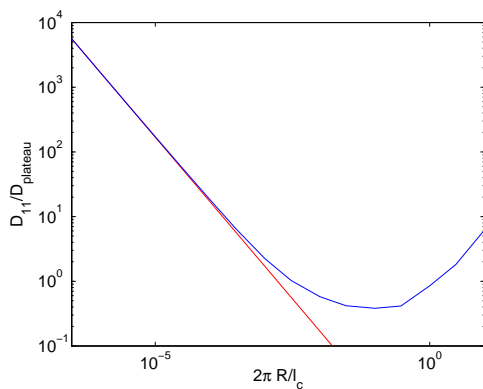


Fig. 5: Normalized diffusion coefficient for W7-AS; red - asymptotic value.

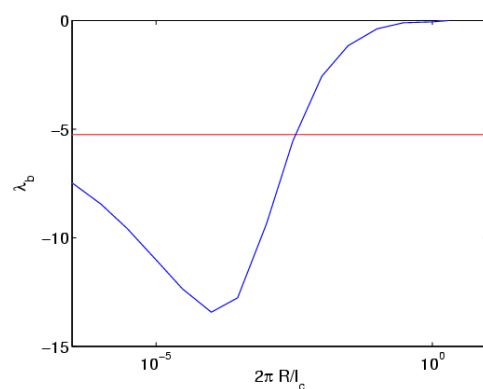


Fig. 6: Bootstrap coefficient for W7-AS; red - asymptotic value.