Monte Carlo δf Simulations of Neoclassical Phenomena in Tokamak Plasmas

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Abstract. The following neoclassical phenomena are studied with drift-kinetic simulations: The bootstrap current inside an island caused by a helical field perturbation, the polarization current in a rotating island, and the bootstrap current caused by a large density or temperature gradient. The first two topics are important for the theory of the neoclassical tearing mode (NTM). The δf code HAGIS with pitch angle collisions modelled by a Monte Carlo procedure is used, and only the ion motion is studied, since the focus is on the effects of finite orbit size. We find that the *ion bootstrap current in small islands* does not vanish; the full unperturbed current is preserved if the island width is smaller than the orbit width. This result leads to a new possible explanation of the scaling of the normalized beta at the onset of the NTMs in ASDEX-Upgrade. The *ion polarization current* caused by the rotation of the island is found to be close to the low-collisionality limit within a large range of collisionalities. It is strongly reduced compared to the thin-orbit theory result if the island half-width is smaller than the banana orbit width. In the absence of an island the *bootstrap current due to a large gradient* with a gradient length of order the banana orbit width or smaller is also reduced as compared to the standard neoclassical theory, and it depends non-locally on the gradients.

1. Introduction and numerical model

Neoclassical phenomena play an important role in present ITER relevant tokamak experiments and will do so in ITER [1,2]. They arise by the interplay of the Coulomb collisions among the particles and the peculiar particle orbits in the non-uniform magnetic field. Although a reliable analytic theory of neoclassical phenomena exists, in specific cases when basic ordering assumptions of the theory are not valid, numerical calculations that do not require the smallness of certain ordering parameters are necessary. We study three topics that involve finite-size ion orbits with drift-kinetic particle simulations:

(i,ii) The currents that drive neoclassical tearing modes (NTM): The (lack of) bootstrap current inside the island, and the neoclassical polarization current which is strongly enhanced over the classical value by the existence of trapped particle orbits. Here, the conventional theory is likely to fail if the banana orbit width is not small compared to the width of the island. The polarization current is the main topic of this article.

(iii) the bootstrap current due to a steep density (temperature) profile.

The numerical simulations are performed with the guiding-centre δf code HAGIS[3], in which the deviation δf of the distribution function from a prescribed Maxwellian is represented by marker particles whose equations of motion are solved in Boozer's magnetic coordinates. The pitch angle part of the Fokker-Planck collision operator with the proper velocity dependence is modelled by a Monte Carlo procedure[4].

An analytically defined equilibrium with flux surfaces with circular cross section and the following profile of the safety factor, $q = 1 + 2\psi/\psi_a$, is used for the simulations (ψ is the poloidal flux, and ψ_a its value at the minor radius). For the studies of the current in an island a single helical perturbation to the poloidal flux, $\hat{\psi} \cos \xi$ is assumed, where $\xi = m\theta - n\zeta + \omega t$ is a helical angle, m = 3 and n = 2 are the poloidal and toroidal mode numbers, ω is the island rotation frequency. This perturbation produces an island with half-width $w_{\psi} = w \frac{d\psi}{dr} = (3\psi_a \hat{\psi})^{1/2}$. The banana orbit width is denoted by $\rho_b = q\rho_i/\varepsilon^{1/2}$, ρ_i is the ion gyro radius and $\varepsilon = r/R$.

2. The bootstrap current in the island of a NTM

Neoclassical tearing modes (NTM) have been shown to limit the maximum achievable β in many tokamak experiments[1]. They are helical perturbations to the equilibrium magnetic field creating an island structure thus connecting along the field lines volume elements with different radii. The neoclassical contribution to the rate of change of the island half-width w is proportional to an integral over the helical part of the parallel current,

$$\frac{dw}{dt}\Big|_{\rm neo} \sim \frac{1}{w} \int_{-1}^{\infty} d\Omega \iint \frac{j_{\parallel \rm neo} \cos \xi}{\sqrt{\Omega + \cos \xi}} \, d\xi d\theta,\tag{1}$$

where $\Omega = 2(\psi - \psi_s)^2/w_{\psi}^2 - \cos \xi$ is a normalized helical flux, $\Omega = 1$ (-1) defines the island separatrix (O point), and the index s denotes the resonant surface. One contribution to the current $j_{\parallel neo}$ is the reduction of the bootstrap current due to the flattening of the pressure profile inside the island which is effectively a current in the opposite direction. The theory of NTMs assumes complete flattening of the pressure profile over the width of the island, and consequently, a complete loss of the bootstrap current implying a maximum drive of the mode. However, banana orbits with their finite width can partly overlap with the interior of the island and with the plasma outside the island. Thus there can be a pressure gradient across these orbits and, in small islands, this leads to a non-zero current inside the island. This current is carried by ions, since the electrons have a much smaller banana orbit width.

We find that the ion bootstrap current inside the island vanishes only if the island is big, but there is a finite current if the island is sufficiently small[5]. This is demonstrated in Fig. 1 where the bootstrap current in islands with normalized half-widths of $w = 9\rho_b$ and $w = 0.6\rho_b$ is depicted. The full ion bootstrap current of the unperturbed equilibrium is preserved if the island width is smaller than the banana orbit width, $\rho_b/w \gtrsim 1$. This effect sets a lower limit to the size of the seed island of a NTM. For the current in the island we obtain the relation[5] $j_{isl}/j_{unpert} = 7(\rho_b/w)^2/(1 + 7(\rho_b/w)^2)$ (Fig. 2) which leads to a new explanation of the linear dependence of β_N^{onset} (the normalized beta at the onset of an almost saturated NTM) on ρ_p^* (the normalized poloidal gyro radius) that was observed in ASDEX Upgrade[6] without a need to recur to a stabilizing effect of the polarization current or the finite perpendicular transport.



Fig. 1 (l.h.s. and centre). The bootstrap current in the presence of an island. The island half-widths are $w = 9\rho_b$ and $w = 0.6\rho_b$, $\rho_b = q\rho_i/\varepsilon^{1/2}$ is the banana orbit width.

Fig. 2 (r.h.s.). The bootstrap current in the island (normalized to the current present without island) versus the ratio between orbit width ρ_b and island half-width w. Solid curve: $j_{\rm isl}/j_{\rm unpert} = 7(\rho_b/w)^2/(1+7(\rho_b/w)^2)$.

3. The polarization current of a rotating island

Since the islands of NTMs rotate, there is a time-dependent electric field which consists of two contributions: the first part is to leading order directed perpendicular to the helical flux surfaces, rotates with the island and vanishes inside. The second part is perpendicular to the unperturbed flux surfaces; it causes the plasma to rotate with the island and is cancelled by the other part far away from the island where the plasma is at rest. In the simulations an electric potential of the form[7]

$$\Phi = -\frac{q\omega}{m} \left\{ (\psi - \psi_s) - \operatorname{sign}(\psi - \psi_s) \frac{w_{\psi}}{\sqrt{2}} (\sqrt{\Omega} - 1) \Theta(\Omega - 1) \right\}$$
(2)

is prescribed (with $\Theta(x) = 1$ for x > 0, $\Theta(x) = 0$ for x < 0). The resulting electric field along a radius through the O-point of the island is shown in Fig. 4. Outside the separatrix the electric field has a scale length proportional to the island width. The first consequence of the radial electric field E_r is a parallel flow of magnitude[7] $u_{\parallel} = \langle E_r/B_p \rangle$ (the brackets denote the flux surface average, B_p is the poloidal magnetic field), because the trapped particles cannot follow on average the poloidal $E \times B$ rotation, and by collisions the rotation of the passing particles is damped, too. In Fig. 3. the parallel flow (steady state after many collision times) is shown for three cases with islands of different sizes. Evidently, if the island width is not large compared to the orbit width, the parallel flow is reduced inside the island and spread out to the plasma outside the separatrix; hence, the relation $u_{\parallel} = \langle E_r/B_p \rangle$ is not valid then. In the central plot of Fig. 3 also the current carried by the trapped particles is shown to be smaller by a factor $\varepsilon^{3/2}$.

The second effect of the time-dependent electric field is a polarization current across flux surfaces which is strongly enhanced over the classical value $nm_i\dot{E}_r/B^2$ due to the finite banana orbit width. According to the analytic theory [7], in the collisional regime $\nu \gg \omega$ it is $j_p = (nm_i/B_p) du_{\parallel}/dt$, the enhancement factor is q^2/ε^2 . In the low-collisionality regime, the parallel flow is to leading order constant on the flux surface, only the next order contribution leads to a polarization current which is smaller by a factor $\varepsilon^{3/2}$. The polarization current is carried by the ions since their orbits have a much larger radial extent than the electron orbits, and it is closed by electron currents parallel to the magnetic field which contribute to the current in the integral in Eq.(1) which drives the NTM. This parallel current is related by $\nabla_{\parallel} j_{\parallel} = -\nabla_{\perp} \cdot j_{\perp}$ to the ion current across the flux surface

$$\vec{j}_{\perp} = \int (\vec{v}_d \cdot \frac{\nabla\Omega}{|\nabla\Omega|}) \frac{\nabla\Omega}{|\nabla\Omega|} \,\delta f d^3 \vec{v} = \int \frac{\Omega\nabla\Omega}{|\nabla\Omega|^2} \,\delta f d^3 \vec{v}. \tag{3}$$



Fig. 3. Parallel ion flow in the island (red) compared to $\langle E_r/B_p \rangle$ (blue) and to $E_r/B_p(\xi = 0)$ (green) for different ratios of island size to orbit width. In the central plot also the current carried by the trapped particles is depicted which is smaller by a factor $\varepsilon^{3/2}$.



Fig. 4 (l.h.s.). Electric field along radius through the O-point. Fig. 5 (centre). $I_p = \langle (\nabla_{\perp} \cdot \vec{j}_{\perp}) \sin \xi \rangle$ varies quadratically with the island rotation frequency ω . Fig. 6 (r.h.s.). $I_p / \varepsilon^{3/2}$ versus the ratio of island half-width to banana orbit width. The polarization current in small islands is strongly reduced. (The diamonds depict results for $\omega \ll k_{\parallel} v_{\rm th}$).

Here, $\hat{\Omega}$ is the rate of change of the helical flux Ω along the ion trajectory, a quantity which is calculated in the simulations. Owing to $\int \nabla_{\parallel} j_{\parallel} d\theta = \int k_{\parallel} \frac{\partial j_{\parallel}}{\partial \xi} d\theta$ we can replace ∇_{\parallel} by $k_{\parallel} \partial / \partial \xi$ and the $\cos \xi$ component of j_{\parallel} in Eq.(1) depends on the $\sin \xi$ component of \vec{j}_{\perp} . We calculate the integral

$$\iint \nabla_{\perp} \cdot \vec{j}_{\perp} \frac{\sin \xi \, d\xi d\theta}{\sqrt{\Omega + \cos \xi}} \sim \frac{\partial}{\partial \Omega} \iiint \dot{\Omega} \sin \xi \, \delta f \, \frac{d^3 \vec{v} \, d\xi d\theta}{\sqrt{\Omega + \cos \xi}} \equiv I_p, \tag{4}$$

and take the maximum of $I_p(\Omega)$ which is found near the separatrix. Simulations of rotating islands were performed with different sets of parameters $\nu, \omega, \varepsilon, T_i$ and with flat density and temperature profiles such that no bootstrap current is driven.

In the regime $\omega \gg k_{\parallel}v_{\rm th}$ the quadratic dependence of j_{\perp} and I_p on ω derived in Ref. [7] (note that $\omega_* = 0$) is observed (Fig. 5) as well as $I_p \sim \varepsilon^{3/2}$ for $\nu/\varepsilon \ll \omega$ (Fig. 6). Also, for big islands with $w \gtrsim 2\rho_b$ the scaling $I_p \sim (w/\rho_b)^{-1}$ from the thin-orbit theory[7] is obtained (Fig. 6; note that $I_p \sim \nabla_{\perp} \cdot \vec{j}_{\perp} \sim k_{\parallel} j_{\parallel} \sim w j_{\parallel}$) under the condition $\omega > k_{\parallel} v_{\rm th}$ the derivation in [7] is based on. In the opposite case with $\omega \ll k_{\parallel} v_{\rm th}$ the scaling is more like $I_p \sim (w/\rho_b)^0$ (green diamonds in Fig. 6).

In small islands, however, the polarization current is strongly reduced by a factor proportional to $(w/\rho_b)^2$ (Fig. 6). This implies that in small islands the parallel electron current which short-circuits the ion polarization current is almost independent of the island size instead of increasing like $1/w^2$ in the thin-orbit theory; consequently, the drive for the NTM [Eq.(1)] increases only like 1/w, not like $1/w^3$. This effect strongly reduces for $w < \rho_b$ a possible stabilizing contribution of the polarization current to the island dynamics that so far was considered important just for small islands owing to the $1/w^3$ scaling.

The transition from the low-collisionality limit, $\nu/\varepsilon\omega \ll 1$ to the collisional limit, $\nu/\varepsilon\omega \gg 1$ was also examined. We find that the current is close to the low-collisionality limit within a large range of values of the collisionality up to $\nu/\varepsilon\omega \approx 7$ (Fig. 7), whereas the transition to the collisional limit takes place at a higher collisionality than according to the theory in Ref. [8]. Also, $\nu/\varepsilon k_{\parallel} v_{\rm th} \gg 1$ is required; therefore, in the regime $\nu_* = \nu q R/\varepsilon^{3/2} v_{\rm th} \leq 1$, the collisional limit can only be approached in simulations with small islands ($w \ll \rho_b$).



Fig. 7. Collisionality dependence of the polarization current. Curves: Function $g(\nu/\omega) = (\nu^2/\omega^2 + \varepsilon^{1/2})/(\nu^2/\omega^2 + \varepsilon^{-1})$ [8].

4. The bootstrap current due to a steep density profile

Another important topic is the bootstrap current in the presence of a large density or temperature gradient. Strong gradients exists, e.g. at the position of a transport barrier. The same code, but without the helical perturbation, is used to calculate the bootstrap current in presence of a steep pressure profile. A result according to the standard neoclassical theory[9] is only obtained if the gradient length is long compared to the banana orbit width. If the gradient length is of the order of the orbit width a strong local reduction of the bootstrap current is observed, and the current is spread over a broader radial interval, i.e. the relation between the current and the gradients is non-local (Fig. 8). Furthermore, if ions that cross on their orbits a certain radius are lost (e.g. ions entering a scrape-off layer), then the bootstrap current is strongly reduced near this radius, too (Fig. 9).



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