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High-Z impurities in magnetic confinement devices are prone to develop density variations on the flux-surface, which can significantly affect their transport. In this paper, we generalize earlier analytic stellarator calculations of the neoclassical radial impurity flux in the mixed-collisionality regime (collisional impurity and low-collisionality bulk ions) to include the effect of such flux-surface variations. We find that only in the homogeneous density case is the transport of highly collisional impurities (in the Pfirsch-Schlüter regime) independent of the radial electric field. We study these effects for a Wendelstein 7-X (W7-X) vacuum field, with simple analytic models for the potential perturbation, under the assumption that the impurity density is given by a Boltzmann response to a perturbed potential. In the W7-X case studied, we find that larger amplitude potential perturbations cause the radial electric field to dominate the transport of the impurities. In addition, we find that classical impurity transport can be larger than the neoclassical transport in W7-X.

1. Introduction

At fusion-relevant temperatures, heavy impurities in high ionisation states, “high-Z impurities”, emit a significant amount of radiation, and even a tiny fraction of impurity ions radiate enough power to seriously challenge the power balance in a reactor. High-Z impurities thus cannot be allowed to accumulate in the center of a magnetic-confinement fusion reactor.

In tokamaks, impurities are expelled from the core of the reactor by neoclassical transport if their temperature gradient is sufficiently large – a situation known as temperature screening. In stellarators, the outlook has been more pessimistic, as the radial transport is not independent of the radial electric field, and an inward pointing electric field is predicted for a stellarator reactor, which would transport impurities inwards [Hirsch et al. 2008].

Recent analytical results on neoclassical stellarator impurity transport have however shown that when the plasma is in a mixed-collisionality regime – where the bulk ions are at low collisionality (1/ν or √ν regimes) and the impurity ions are collisional – the radial impurity flux becomes independent of the electric field, which allows temperature screening to be effective in stellarators [Newton et al. 2017; Helander et al. 2017]. This is due to a cancellation between the flux driven by impurity parallel flow and

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the ion thermodynamic forces. Similar cancellation is also found in the regimes where both ions and impurities are collisional (Braun & Helander 2010), although in this case, thermodiffusion is usually inward unless the effective charge is very small, so no temperature screening occurs (Rutherford 1974).

However, high-Z impurities are also sensitive to flux-surface variations in the electrostatic potential, in response to which they can develop density variations on flux-surfaces. Such variations can have large effects on the neoclassical transport, as has been demonstrated analytically (Angioni & Helander 2014; Calvo et al. 2018) and numerically (Angioni et al. 2014; García-Regaña et al. 2017; Mollén et al. 2018) for tokamaks and stellarators. For the effects on turbulent transport in tokamaks, see for example Mollén et al. (2012, 2014); Angioni et al. (2014).

In this work, we generalize the analytical calculation in (Newton et al. 2017) to account for flux-surface variation of the impurity density in stellarators, using a fluid description for the impurities and solving for the ion distribution function in the $1/\nu$ regime. Our expression for the impurity flux agrees with that in Calvo et al. (2018), where the same problem is treated fully kinetically. Like Calvo et al. (2018), we find that the effect of the radial electric field can be large when the amplitude of the flux-surface variation is large. In addition, we find that classical transport can be dominant compared to the neoclassical transport for collisional impurities in certain stellarator geometries.

The remainder of this paper is organised as follows: in Sec. 2 we present the equations describing the impurities, and relate the friction force acting on the impurities to their flux-surface density variations and the resulting radial flux. In Sec. 3 we introduce the ion-impurity collision operator and obtain an explicit expression for the ion-impurity friction force. In Sec. 4, we consider simplifying limits of the equations presented in the previous sections, and derive expressions for transport coefficients in those limits. Sec. 5 treats the classical transport, and shows why it is important in Wendelstein 7-X. Finally, in Sec. 6, we apply our results to study a test-case based on a Wendelstein 7-X vacuum field.

### 2. Impurity equations

In this section, we present equations to model the impurities, starting from momentum balance and ending with expressions for calculating the flux along the magnetic field and across the flux-surface.

The impurities are assumed to be collisional enough to be in the Pfrish-Schlüter regime and thus have a Maxwellian velocity distribution, with the density not necessarily constant on flux-surfaces. For such a species in steady-state, the momentum equation is

$$\nabla p_z = Zen_z E + Ze \Gamma_z \times B + R_z$$

where the $z$ species subscript refers to the impurities, $Z$ is the impurity charge-number, $e$ the proton charge, $p_z$ the impurity pressure, $n_z$ the impurity density, $\Gamma_z$ the impurity particle flux, $B$ the magnetic field, $E$ the electric field, and $R_z$ is the friction force acting on the impurities. By projecting (2.1) onto the magnetic field direction $b = B/|B|$, we obtain

$$\nabla \parallel p_z = Zen_z E \parallel + R_z \parallel.$$  

From (2.2), we see that pressure (and thus density) variation along the field-line is set up by forces associated with the parallel electric field and friction – both of which increase with the impurity charge number. The friction force can be calculated using kinetic
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information of all other species, as

$$R_z = m_z \sum_a \int d^3 v \nu C[f_z, f_a],$$

(2.3)

where $f_a$ is the distribution function of a species “a”. We will restrict ourselves to the case where only collisions between a bulk ion species $i$ and the impurities matter: the electron contribution to the friction force can be neglected as small in the electron-ion mass ratio.

In order to simplify the kinetic calculations required to determine $f_i$, we will assume that $Z \gg 1$, so that the effects that lead to pressure variation on the flux-surface are small for the bulk ions. In the $Z \gg 1$ limit, the ions and impurities will have undergone temperature equilibration if [Helander 1998]

$$\frac{\rho_s \tilde{\nu}_{ii}}{Z} \ll 1,$$

(2.4)

where $\rho_s = \rho_i/L$, with $L$ the profile length-scale and $\rho_i = v_{T_i} m_i/eB$ the ion thermal gyroradius, with $m_i$ the ion mass and $v_{T_i} = \sqrt{2 T_i/m_i}$ the ion thermal speed; $\tilde{\nu}_{ii} = n_i e^4 \ln \Lambda L_{\parallel}/(T_i^2 e_0^2 12 \pi^{3/2})$ is the ion collisionality where $L_{\parallel}$ is the length-scale of the $n_z$- and $\Phi$-variations parallel to $B$; $e_0$ the vacuum permittivity and $\ln \Lambda$ the Coulomb-logarithm. Equation 2.4 is practically always satisfied in a magnetized plasma, so we will assume that $T_z = T_i$ is a flux-function, and (2.2) thus becomes an equation for the flux-surface variation of $n_z$.

Furthermore, if $\Delta \equiv Z^2 \rho_s \tilde{\nu}_{ii} \ll 1$, as in the conventional drift-kinetic ordering, the friction force in (2.2) becomes smaller than the other terms [Helander 1998]. To zeroth order in $\Delta$, the density in (2.2) is then given by a Boltzmann response to $\Phi$

$$n_z = N_z e^{-Ze\Phi/T_z}, \quad (\Delta \ll 1)$$

(2.5)

where $N_z$ is a flux-function. If the density variation of all species is given by (2.5), quasi-neutrality forces the density to also be a flux-function. For significant density variation to arise on a flux-surface, one of these assumptions thus has to be violated; several different mechanisms have been considered in the literature:

In [Helander 1998], $\Delta = \mathcal{O}(1)$, so the impurities themselves set up their own flux-surface variation to balance the flux-surface variation of the friction force and electric field. This was generalized in [Fülöp & Helander 1999] to include centrifugal forces.

Heating can introduce a fast particle population, which may not have a density variation according to (2.5) and thus leads to an electric field tangential to the flux surface, which the impurity density in (2.2) responds to. Such effects were considered in [Kazakov et al. 2012] and [Angioni & Helander 2014], and are often more important than the variations set up by the impurities themselves.

Furthermore, in stellarators, helically trapped particles drifting due to the radial electric field can cause an in-out density asymmetry that, in turn, causes an electric field [García-Regaña et al. 2017]. This electric field then affects the impurities. This mechanism has been investigated numerically in [García-Regaña et al. 2017], and was found to significantly affect the transport in the Large Helical Device (LHD) and TJ-II stellarators, but does not appear to have a major effect in Wendelstein 7-X (W7-X) due to the neoclassical optimization reducing the radial extent of such helically trapped orbits.

To be able to treat all of these scenarios, we will allow $\Phi$ and $\Delta$ to be arbitrary, as long as the tangential variation in $\Phi$ (which we denote by $\tilde{\Phi}$), is of magnitude $e\tilde{\Phi}/T_i \sim Z^{-1}$.
so that its effect can be neglected for the bulk ions. In Sec. 4, we will consider the case when \( \Delta \ll 1 \) with \( \Phi \) set by fast particles.

2.1. Radial impurity flux

Regardless of the mechanisms that determine the spatial variation of \( n_z \), we can calculate the perpendicular flux of the Maxwellian impurities by applying \( B \times \) to (2.1), resulting in

\[
\mathbf{B} \times \nabla p_z = \mathbf{B} \times Z n_z \mathbf{E} + Z e B^2 \mathbf{T}_{z, \perp} + \mathbf{B} \times \mathbf{R}_z. \tag{2.6}
\]

This expression contains the flux in both the diamagnetic and radial directions. The flux-surface averaged radial flux becomes

\[
Ze \left< \mathbf{\Gamma}_z \cdot \nabla \psi \right> = \left< \mathbf{B} \times \nabla \psi \cdot \mathbf{R}_z \right> + Ze \left< n_z \frac{\mathbf{B} \times \nabla \psi}{B^2} \cdot \mathbf{E} \right> - \left< \frac{\mathbf{B} \times \nabla \psi}{B^2} \cdot \nabla p_z \right>, \tag{2.7}
\]

where \( \psi \) is an arbitrary flux-surface label and \( \left< \cdot \right> \) denotes the flux-surface average. Here, the first term on the right is the classical flux, and the second one is the radial flux due to the \( \mathbf{E} \times \mathbf{B} \)-drift. As there is no radial current in steady-state (i.e. \( \nabla \times \mathbf{B} \cdot \nabla \psi = 0 \)), we have

\[
\left< \mathbf{B} \times \nabla \psi \cdot \nabla X \right> = 0 \tag{2.8}
\]

for any single-valued function \( X \). The last term of (2.7) can thus be rewritten as \( \left< p_z \mathbf{B} \times \nabla \psi \cdot \nabla B^{-2} \right> \), which is the radial flux due to the magnetic drift of a Maxwellian species. Thus the two latter terms in (2.7) correspond to the neoclassical flux, and will be denoted by \( \left< \mathbf{\Gamma}_z \cdot \nabla \psi \right>^{\text{NC}} \).

From this point, we will assume that the inductive electric field is small, so that \( \mathbf{E} = -\nabla \Phi \). Following Calvo et al. (2018), we obtain a flux-friction relation by introducing two functions, \( u \) and \( w \), defined through the magnetic differential equations

\[
\mathbf{B} \cdot \nabla u = -\mathbf{B} \times \nabla \psi \cdot \nabla B^{-2}, \tag{2.9}
\]

\[
\mathbf{B} \cdot \nabla (n_z w) = -\mathbf{B} \times \nabla \psi \cdot \nabla (n_z B^{-2}), \tag{2.10}
\]

so that

\[
Ze \left< \mathbf{\Gamma}_z \cdot \nabla \psi \right>^{\text{NC}} = \left< \mathbf{B} \cdot [Z n_z \nabla \Phi + u \nabla p_z] \right> = \left< \mathbf{B} \cdot [(u - w) \nabla p_z + w \mathbf{R}_z] \right>, \tag{2.11}
\]

where we have used parallel force-balance to eliminate the parallel electric field from the expression. We can thus evaluate the neoclassical transport for a given \( n_z \), provided that \( \left< w B R_{z \parallel} \right> \) is known in terms of \( n_z \); such an expression for \( R_{z \parallel} \) is presented in Sec. 3. To calculate the friction force, we must however know the parallel impurity flux, which is the subject of the next section.

2.2. Parallel impurity flux

From (2.6), we get the impurity flux in the \( \mathbf{B} \times \nabla \psi \)-direction (denoted with a \( \wedge \) subscript) as

\[
\mathbf{\Gamma}_z \wedge = \frac{\mathbf{B} \times \nabla \psi}{Ze B^2} \left( Z n_z \frac{\partial \Phi}{\partial \psi} + \frac{\partial p_z}{\partial \psi} + \frac{\mathbf{R}_z \cdot \nabla \psi}{|\nabla \psi|^2} \right). \tag{2.12}
\]

† Note that Calvo et al. (2018) defines \( U_1 \) instead of \( w \); they are related through \( U_1 = wn_z/N_z \).
In a confined plasma, the radial fluxes and thus the radial friction will be small, so we can neglect \( R_z \cdot \nabla \psi \) in (2.12) and neglect the radial flux in the impurity continuity equation \( \nabla \cdot \Gamma_z = 0 \). The parallel impurity flux \( \Gamma_{z,\|} \) thus satisfies

\[
B \cdot \nabla \left( \Gamma_{z,\|} B^{-1} \right) = -\nabla \cdot \Gamma_{z,\perp}.
\] (2.13)

In (2.12), the second term will be much smaller when \( Z \gg 1 \), unless \( p_z \) varies on scales \( Z \) times shorter than \( \Phi \), which is never the case in practice. In the \( Z \gg 1 \) limit, (2.13) thus becomes (recalling \( e\Phi/T \sim Z^{-1} \))

\[
B \cdot \nabla \left( \Gamma_{z,\|} B^{-1} \right) = -\nabla \cdot \Gamma_{z,\perp} \cdot \nabla \left( \frac{n_z}{B^2} \right)
\] (2.14)

so that

\[
\Gamma_{z,\|} \equiv n_z V_{z,\|} = wn_z \frac{d \langle \Phi \rangle}{d\psi} B + BK_z,
\] (2.15)

where \( K_z(\psi) \) is an integration constant.

### 3. Parallel friction force

With the parallel impurity flux from the previous section, we now have everything needed to calculate the ion-impurity parallel friction.

As the collisions with electrons can be neglected, the friction force on the impurities can be expressed as

\[
R_z \approx R_{zi} = -R_{iz} = - \int d^3 v m_i \nu C_{iz},
\] (3.1)

where \( R_{ab} \) denotes the friction force on species \( a \) by species \( b \), and \( C_{iz} \) is the ion-impurity collision operator. Since \( m_z \gg m_i \) for high-Z impurities, we can use a mass-ratio expanded ion-impurity collision operator

\[
C_{iz} = \nu_{iz}^D(v) \left( \mathcal{L}(f_{i1}) + \frac{m_i v \cdot V_z}{T_i} f_{i0} \right),
\] (3.2)

where \( V_z = \Gamma_z/n_z \) is the flow of the impurities, \( \mathcal{L} \) is the Lorentz operator (Helander & Sigmar 2005), \( f_{i1} \) the order \( \rho^* \) part of the ion distribution function, and the collision frequency \( \nu_{iz}^D \) is

\[
\nu_{iz}^D = \frac{n_z Z^2 e^4 \ln \Lambda}{4\pi m_i^2 \epsilon_0^2 v^3}.
\] (3.3)

The lowest order ion distribution function \( f_{i0} \) is taken to be a stationary Maxwell-Boltzmann distribution, and to calculate the parallel friction force we only need the gyrophase-independent part of \( f_{i1} \) (which we denote by \( F_{i1} \)). This function is given by the ion drift-kinetic equation

\[
v_{\|} \nabla_{\|} F_{i1} + v_d \cdot \nabla f_{i0} = C_i,
\] (3.4)

where gradients are taken with \( \mathcal{E} = mv^2/2 + e\Phi \) and \( \mu = m_i v_\perp^2/(2B) \) fixed – although we will later make use of the fact that the potential energy is approximately constant over an ion orbit and use the approximate invariants \( v \) and \( \lambda = v_\perp^2/(v^2 B) \) as velocity coordinates.

The collision operator is approximately given by collisions with bulk ions and impurities, \( C_i \approx C_{iz} + C_{ii} \), and we use a model operator for ion-ion collisions

\[
C_{ii} = \nu_{ii}^D(v) \left( \mathcal{L}(F_{i1}) + \frac{m_i v \cdot U}{T_i} f_{i0} \right),
\] (3.5)
where $\mathbf{U}$ is determined by momentum conservation and the collision frequency is

$$v_{\text{ii}}^D = \frac{n_i e^4 \ln A}{4\pi m_i^2 \epsilon_0 v_i^3} \left( \text{erf} \left( \frac{v}{v_{T_i}} \right) - G \left( \frac{v}{v_{T_i}} \right) \right),$$

(3.6)

where erf is the error function and $G$ the Chandrasekhar function \cite{helander2005}. We will assume that $C_i$ is smaller than the other terms in (3.4) and expand $F_{i1} = F_{i1}^{(0)} + F_{i1}^{(1)} + \ldots$ in collisionality, so that

$$v\parallel \nabla F_{i1}^{(0)} + \mathbf{v}_d \cdot \nabla f_i = 0 \quad (3.7)$$

$$v\parallel \nabla F_{i1}^{(1)} = C_i [F_{i1}^{(0)}].$$

(3.8)

We solve (3.7) and (3.8) as in \cite{newton2017}, except that we allow $n_z$ to vary on the flux-surface, which makes the expressions less compact; the details are thus relegated to appendices A–D.

The parallel friction force becomes

$$R_{iz\parallel} = \tau_{iz\parallel} \frac{\tau_i z}{n_i m_i} = \left[ w - \frac{\langle wB^2 \rangle}{\langle B^2 \rangle} \right] B \frac{d\langle \Phi \rangle}{d\psi} + \left[ \frac{1}{n_z} - \frac{\langle B^2 \rangle}{\langle B^2 \rangle} \right] BK_z$$

$$- \left[ u - \frac{\langle uB^2 \rangle}{\langle B^2 \rangle} \right] B \frac{T_i}{e} \left[ A_{i1} - \frac{3}{2} A_{i2} \right],$$

(3.9)

where $A_{i1} = \frac{d \ln p_i}{d\psi} + \frac{e \langle \Phi \rangle}{T_i \frac{d\psi}{d\psi}}$ and $A_{2i} = \frac{d \ln T_i}{d\psi}$ are the ion thermodynamic forces; $\tau_{iz}^{-1} = Z^2 n_z e^4 \ln A / (3\pi^{3/2} m_i^2 \epsilon_0 v_i v_{T_i}^3)$; $K_z$ is determined by the solvability condition on (2.2), $\langle n_z^{-1} BR_{iz\parallel} \rangle = 0$, and is given by

$$K_z(\psi) = - \left\langle \frac{B^2}{n_z} \left( 1 - c_4 \alpha \right) \right\rangle^{-1} \frac{d\langle \Phi \rangle}{d\psi} \langle (1 - c_4 \alpha) wB^2 \rangle$$

$$+ \left\langle \frac{B^2}{n_z} \left( 1 - c_4 \alpha \right) \right\rangle^{-1} \left( c_1 a_2 + b_2 + \langle uB^2 \rangle [c_1 + 1] \right) T_i \frac{T_i}{e} A_{i1}$$

$$+ \left\langle \frac{B^2}{n_z} \left( 1 - c_4 \alpha \right) \right\rangle^{-1} \left( c_1 \left[ a_3 - \frac{5}{2} a_2 \right] + \left[ b_3 - \frac{5}{2} b_2 \right] - \langle uB^2 \rangle \left[ c_1 \eta + \frac{3}{2} \right] \right) T_i \frac{T_i}{e} A_{i2},$$

(3.10)

where $\alpha = Z^2 n_z / n_i$; $\eta \approx 1.17$; the $a_i$, $b_j$ and $c_k$ are flux-surface constants which depend on the magnetic geometry and the impurity density variations on the flux-surface, and are defined in equations (C3)–(C6), (B4)–(B5), and (D3)–(D4) in the appendices.

3.1. Trace impurity limit

In the trace impurity limit, $\alpha \ll 1$, all the non-standard flux-surface constants -- $a_i$, $b_j$ and $c_k$ -- reduce to known functions that only depend on the magnetic geometry, see
The resulting friction force is

$$R_{iz,∥} = \frac{\tau_{iz}}{n_i m_i} = \left( w - \left\langle w B^2 \right\rangle \right) B \frac{d \langle \Phi \rangle}{d \psi}$$

$$+ \left( \left\langle u B^2 \right\rangle - u + \left( \frac{1}{n_z \left\langle B^2 \right\rangle} - \frac{1}{\left\langle B^2 \right\rangle} \right) \left[ f_s + \left\langle u B^2 \right\rangle \left( \frac{f_c}{1 - f_c} + 1 \right) \right] \right) B \frac{T_i}{e} A_{i1}$$

$$- \left( \frac{3}{2} \frac{\left\langle u B^2 \right\rangle}{\left\langle B^2 \right\rangle} - \frac{3}{2} u + \left( \frac{1}{n_z \left\langle B^2 \right\rangle} - \frac{1}{\left\langle B^2 \right\rangle} \right) \left[ f_s + \left\langle u B^2 \right\rangle \left( \frac{\eta f_c}{1 - f_c} + \frac{3}{2} \right) \right] \right) B \frac{T_i}{e} A_{i2},$$

where $f_c$ and $f_s$ are defined in (E7) and (E8). Equation 3.11 can be used to solve for $n_z$ from the parallel momentum equation (2.2), given a mechanism to set $\tilde{\Phi}$. We will not attempt such a daunting task at this time, and instead consider simplifying limits in the following section.

4. $\Delta \ll 1$ limit

In the $\Delta \ll 1$ limit, with $n_z = n_{z0} + n_{z1} + \ldots$, the zeroth-order parallel momentum equation becomes

$$T_z \nabla_{∥} n_{z0} = -Ze n_{z0} \nabla_{∥} \Phi,$$

so the zeroth order impurity density is given by a Boltzmann response to $\Phi$

$$n_{z0} = N_z(\psi) e^{-Ze \Phi / T_z},$$

where $N_z$, sometimes referred to as the pseudo-density, is a flux-function. Here, we assume that $\tilde{\Phi}$ is known. This corresponds to $\tilde{\Phi}$ being set by a mechanism unrelated to $n_z$. This is appropriate in the trace limit, as $Z^2 n_z \ll n_i$ so that $Z n_z$ can be neglected in the quasi-neutrality relation, which would otherwise relate $\tilde{\Phi}$ and $n_z$.

If (2.5) is used to write $\Phi$ in terms of $n_{z0}$, the first-order parallel momentum equation becomes

$$T_z n_{z0} \nabla_{∥} \left( \frac{n_{z1}}{n_{z0}} \right) = R_{z∥}[n_{z0}],$$

which has the solvability condition $\langle n_{z1}^{-1} BR_{z∥}[n_{z0}] \rangle = 0$. This is the same solvability condition as that of the exact equation (2.2), except with $n_z \rightarrow n_{z0}$, and thus the friction force in (3.11) can be used with $n_z \rightarrow n_{z0}$ without introducing any errors that destroy the solvability of (4.3).

From (4.3) and (3.11), $n_{z1}$ can now be obtained numerically for a given $\Phi$ or $n_{z0}$. This is however not required to calculate the flux, as it is enough to know $\nabla_{∥} n_{z1}$ to calculate the radial flux from (2.11), which gives

$$\langle \Gamma_z \cdot \nabla \psi \rangle^{NC} = \frac{1}{Ze} \left\langle w_0 BR_{z∥} \right\rangle,$$

where $w_0$ is given by (2.10) but with $n_z \rightarrow n_{z0}$.
Inserting (3.11) into (4.4), the radial flux becomes

\[
\frac{\tau_{i0} n_{i0}}{n_i m_i} \langle w_0 B R_{i\|} [n_{i0}] \rangle = \left( \frac{\langle w_0 B^2 \rangle^2}{\langle B^2 \rangle} - \frac{\langle n_{i0} w_0^2 B^2 \rangle}{\langle B^2 \rangle} \right) \frac{d}{d\psi} \langle \Phi \rangle + \frac{T_i}{e} \left( A_{i1} - \frac{3}{2} A_{i2} \right) \frac{\langle w_0 B^2 \rangle}{\langle B^2 \rangle} \left( f_s + \frac{\langle u B^2 \rangle}{\langle B^2 \rangle} \right) \frac{T_i}{e} \left( 1 - \frac{f_c}{f_c} \right) [A_{i1} - \eta A_{i2}] + \left[ A_{i1} - \frac{3}{2} A_{i2} \right],
\]

which we can decompose into parts driven by density, temperature and potential gradients

\[
\langle \mathbf{T}_z \cdot \nabla \psi \rangle_{NC} = D_{\Phi}^{NC} \frac{e}{T_i} \frac{d}{d\psi} \langle \Phi \rangle - D_{n_i}^{NC} \frac{d \ln n_i}{d\psi} - D_{T_i}^{NC} \frac{d \ln T_i}{d\psi},
\]

where

\[
D_{\Phi}^{NC} = \frac{n_i m_i}{n_{i0} \tau_{i0} Z e} \frac{T_i}{e} \left( \frac{\langle w_0 B^2 \rangle^2}{\langle B^2 \rangle} - \frac{\langle n_{i0} w_0^2 B^2 \rangle}{\langle B^2 \rangle} + \frac{\langle n_{i0} w_0 u B^2 \rangle}{\langle B^2 \rangle} - \frac{\langle u B^2 \rangle}{\langle B^2 \rangle} \right) \frac{\langle n_{i0} w_0 B^2 \rangle}{\langle B^2 \rangle} + \frac{\langle w_0 B^2 \rangle}{\langle B^2 \rangle} - \frac{\langle w_0 B^2 \rangle}{\langle B^2 \rangle} \left( f_s + \frac{\langle u B^2 \rangle}{\langle B^2 \rangle} \right) \frac{1}{1 - \frac{f_c}{f_c}} \left( A_{i1} - \frac{3}{2} A_{i2} \right)
\]

\[
D_{n_i}^{NC} = -\frac{n_i m_i}{n_{i0} \tau_{i0} Z e} \frac{T_i}{e} \left( \frac{\langle n_{i0} w_0 u B^2 \rangle}{\langle B^2 \rangle} - \frac{\langle u B^2 \rangle}{\langle B^2 \rangle} \frac{\langle n_{i0} w_0 B^2 \rangle}{\langle B^2 \rangle} \right) + \frac{\langle n_{i0} w_0 B^2 \rangle}{\langle B^2 \rangle} - \frac{\langle w_0 B^2 \rangle}{\langle B^2 \rangle} \left( f_s + \frac{\langle u B^2 \rangle}{\langle B^2 \rangle} \right) \frac{1}{1 - \frac{f_c}{f_c}} \left( A_{i1} - \frac{3}{2} A_{i2} \right)
\]

\[
D_{T_i}^{NC} = \frac{1}{2} \frac{n_i m_i}{n_{i0} \tau_{i0} Z e} \frac{T_i}{e} \left( \frac{\langle n_{i0} w_0 u B^2 \rangle}{\langle B^2 \rangle} - \frac{\langle u B^2 \rangle}{\langle B^2 \rangle} \frac{\langle n_{i0} w_0 B^2 \rangle}{\langle B^2 \rangle} \right) + \frac{\langle n_{i0} w_0 B^2 \rangle}{\langle B^2 \rangle} - \frac{\langle w_0 B^2 \rangle}{\langle B^2 \rangle} \left( f_s + \frac{\langle u B^2 \rangle}{\langle B^2 \rangle} \right) \frac{1}{1 - \frac{f_c}{f_c}} \left( 1 + (2\eta - 3) f_c \right)
\]

From (4.7), we see that the flux due to the radial electric field is generally non-zero, but that it vanishes when \( n_{i0} \) is constant on the surface. The non-zero \( D_{\Phi}^{NC} \) can in-fact dominate the other neoclassical transport coefficients, as will be seen in Sec. 6.

5. Classical transport

Finally, we calculate the classical flux, given by the first term in (2.7). Using our mass-ratio expanded collision operator and momentum conservation, the perpendicular friction becomes

\[
R_{z_{i\perp}} = -\int d^3 v m_i v_{i\perp} \langle D(v) \rangle \left( v_{i\perp} \mathcal{L}(f_{i1}) + \frac{m_i v_{i\perp} \cdot V_z}{T_i} f_{i0} \right),
\]

where \( v_{\perp} = v - v_{\parallel} b \) with \( v_{\parallel} = v \cdot b \).

In (5.1), only the gyrophase-dependent part of \( f_{i1} \) contributes to the first term, and
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only the perpendicular impurity flow contributes to the last. The gyrophase dependent part of \( f_{i1} \) (which we denote \( \tilde{f}_{i1} \)) is given by Hazeltine (1973)

\[
\tilde{f}_{i1} = -\rho_i \cdot \nabla f_{i0},
\]

(5.2)

where the gyroradius vector is

\[
\rho_i = \rho_i (e_2 \cos \gamma + e_3 \cos \gamma) = b \times v_\perp / \Omega_i,
\]

(5.3)

with \( \{b, e_2, e_3\} \) an orthonormal set of vectors, and \( \Omega_i = eB/m_i \). Thus, we have everything required to calculate the perpendicular friction, which becomes

\[
R_{zi\perp} = \frac{m_i n_i}{n_z \tau_{iz}} B \times \nabla \psi \left[ A_{i1} - \frac{3}{2} A_{i2} \right] - \frac{n_i m_i}{\tau_{iz}} V_z \perp.
\]

(5.4)

Using the same approximations and assumptions as in the neoclassical expressions, we replace \( V_z \perp \) with \( v_E = b \times \nabla \Phi/B \), and thus obtain

\[
R_{zi\perp} = \frac{m_i n_i}{n_z \tau_{iz}} B \times \nabla \psi \left[ \frac{d \ln n_i}{d \psi} - \frac{1}{2} \frac{d \ln T_i}{d \psi} \right],
\]

(5.5)

resulting in the classical impurity flux

\[
\langle \Gamma_z \cdot \nabla \psi \rangle^C = \frac{1}{Ze} \left\langle \frac{B \times \nabla \psi}{B^2} \cdot R_z \right\rangle
\]

(5.6)

or

\[
\langle \Gamma_z \cdot \nabla \psi \rangle^C = -D_{n_i}^C \frac{d \ln n_i}{d \psi} - D_{T_i}^C \frac{d \ln T_i}{d \psi}.
\]

(5.7)

The classical flux is often neglected as smaller than the neoclassical flux. To get a simple estimate of its importance, we take the homogeneous \( n_z \) limit of (4.5) and (5.6), so that the ratio of classical to neoclassical flux depends purely on geometry

\[
\frac{\langle \Gamma_z \cdot \nabla \psi \rangle^C}{\langle \Gamma_z \cdot \nabla \psi \rangle^NC} = \frac{\langle \nabla \psi^2 / B^2 \rangle \langle B^2 \rangle}{\langle u^2 B^2 \rangle \langle B^2 \rangle - \langle u B^2 \rangle^2}.
\]

(5.8)

This ratio is indeed small in conventional tokamaks and stellarators (it is \( \sim 0.1–0.6 \) in ASDEX Upgrade, and \( \sim 0.1–1 \) in LHD), but it is \( \sim 3–3.5 \) in a standard W7-X configuration.

W7-X differs from LHD in that it has been optimized to have a low ratio of parallel to perpendicular current. To see how this affects the ratio (5.8), we can express the parallel current in the following way: Charge conservation imposes \( \nabla \cdot j = 0 \), where \( j \) is the current density. Assuming that the equilibrium magnetic field can be written as \( j \times B = \nabla p \) – where \( p \) is the total pressure \( p = \sum_a p_a \), which is assumed to be a flux-function to the required order – the parallel current density becomes \( j_\parallel = uB \frac{d p}{d \psi} \). The ration of parallel and perpendicular current then becomes

\[
\frac{j_\parallel}{|j_\perp|} = \frac{uB}{B \times \nabla \psi / B^2},
\]

(5.9)

which can be made small by making \( u/|\nabla \psi| \) small, which simultaneously makes (5.8) large. The classical flux remains large even when \( n_z \) varies on the flux-surface, as we will see in the next section.
6. Wendelstein 7-X test case

To explore the implications of the flux-surface variation of $n_{z0}$ in (4.7)–(4.9), we consider a scenario where \( \tilde{\Phi} \) is given by

\[
\tilde{\Phi}(B) = \tilde{\Phi}(B_0)e^{-(B-B_0)^2/(2\sigma^2)},
\]

(6.1)

where \( \tilde{\Phi}(B_0) \) is an amplitude of the potential, \( B_0 \) is an extremum of \( B \), and \( \sigma \) gives the width of \( \tilde{\Phi} \). Equation 6.1 represents a simple case when \( \tilde{\Phi} \) is purely a function of \( B \), which is the expected behaviour when \( \tilde{\Phi} \) is set by fast particles. Specifically, fast, collisionless particles will have distribution functions that only depend on their constants of motions \( \mu \) and \( E \). The resulting fast-particle density then only depends on \( B \) and \( \Phi \),

\[
n_\alpha = \int d^3v f_\alpha(m_\alpha v_\perp^2/2B, m_\alpha v^2/2 + Z_\alpha e\Phi) = n_\alpha(B, \Phi),
\]

(6.2)

where the \( \alpha \) species subscript denotes a fast-particle species. Assuming that the other species have Boltzmann distributed densities, as in (4.2), quasi-neutrality causes \( \Phi \) to be a function of \( B \) and \( \psi \) only.

The size of \( e\tilde{\Phi}/T_i \) is roughly given by the ratio of \( n_\alpha/n_e \). Values of \( e\tilde{\Phi}/T_i \sim 0.05 \) is thus an approximate upper bound; although we are primarily interested in (6.1) as a simple test case, and will not be so concerned with whether it is a realistic fast-particle response.

We take \( B \) from a Wendelstein 7-X vacuum field, and solve the magnetic differential equations for \( u \) and \( w \) numerically for this field. The magnetic field in Boozer coordinates is visualized in Fig. 1 together with an example \( \tilde{\Phi} \) and the resulting \( n_{z0} \) for \( Z = 6 \) and \( \langle n_{z0} \rangle = 10^{17} \text{ m}^{-3} \).

To investigate the effects of a localized \( n_z \) distribution, we performed a scan where the amplitude of the potential perturbation is increased. Specifically, the potential perturbation is centred at \( B_{\text{max}} \) or \( B_{\text{min}} \), and the amplitude \( \tilde{\Phi}(B_0) \) is scanned from \( e\tilde{\Phi}/T_i = -0.1 \) to \( e\tilde{\Phi}/T_i = 0.1 \) – where a negative/positive sign corresponds to impurities accumulating/decumulating at \( B_{\text{max}} \). The ion temperature and density are \( T_i = 1 \text{ keV} \) and \( n_i = 10^{20} \text{ m}^{-3} \).

The resulting transport coefficients are shown in Fig. 2. In the figures, \( D \) (without superscript index) refers to the sum of neoclassical and classical \( D \)'s; for comparison, we also show \( D^{\text{NC}} \). As indicated in Sec. 5, classical transport is dominant for this field configuration, but we also see that the transport due to the radial electric field can be comparable for higher amplitude potential perturbations. We see that both when \( B_0 = B_{\text{max}} \) and \( B_0 = B_{\text{min}} \), there is a narrow amplitude range, roughly \( e\tilde{\Phi}(B_0)/T_i \in [-0.04, 0] \), in which the impurity flux due to an inward radial electric field is weakly
Figure 2: Transport coefficients, for different potential perturbation amplitudes $\Phi(B_0)$, for $\Phi$ localized around (left) $B_{\text{max}}$ and (right) $B_{\text{min}}$. $T_i = 1$ keV and $n_i = 10^{20} \text{m}^{-3}$, $\sigma = 0.1|B_{\text{max}} - B_{\text{min}}|$, $Z = 6$, $\langle n_z \rangle = 10^{17} \text{m}^{-3}$; $D_{\text{NC}}$ refers to the neoclassical transport coefficients, while $D$ is the sum of classical and neoclassical. At amplitudes roughly within $e\Phi/T_i \in [-0.04, 0]$, the flux due to an inward radial electric field is outward but very weak.

positive. Within this window, the flux driven by the electric field is largely unaffected by $\Phi(B_0)$, and the impurities will be driven outwards when the temperature gradient is strong enough, i.e. we have temperature screening. Specifically, temperature screening occurs when $d\psi \ln T_i \gtrsim 2d\psi \ln n_i$, and the magnitude of the flux can be affected by changing the strength of the impurity variation on the flux-surface, but $D_{n_i}/D_{T_i} \approx -2$ to within 1%. At higher potential amplitudes, the radial electric field starts to play a role, but it remains subdominant for realistic amplitudes $e\Phi/T_i \lesssim 0.05$.

From Fig. 2 we also see that most of the variation in $D_{n_i}$ and $D_{T_i}$ comes from the neoclassical flux. This can partly be understood from the simpler form of the classical flux (5.6), where the dependence on $n_z$ is linear, so that the localized $n_z$ perturbation due to $\Phi$ merely acts as a weight in the geometric factor $\langle n_z |\nabla \psi|^2/B^2 \rangle$, which here gives a small effect when integrated over the flux-surface. In contrast, the neoclassical flux (4.5) is non-linear in $n_z$, and the total flux through the flux-surface is set by a balance between inward and outward fluxes at different points on the flux-surface.

To investigate the effects of more localized fast ions, we scanned the width of $\Phi$, while keeping $\langle \Phi \rangle$ and $\langle n_z \rangle$ constant. For small $\sigma$, this results in $n_{z0}$ that are very localized around the extremum of $B$. The result is shown in Fig. 3. From the figure, we see that $D_{\Phi}^{\text{NC}}$ diverges for localized $n_{z0}$. This is due to the $w_0^2$ terms in $D_{\Phi}^{\text{NC}}$: $n_{z0}w_0$ obtained from (2.10) is not localized to regions where $n_{z0}$ is localized, which results in a large $w_0$ where $n_{z0}$ is small. In contrast, the $D_{n_i}^{\text{NC}}$ and $D_{T_i}^{\text{NC}}$ remains finite, as $w_0$ only appears together with an $n_{z0}$ in those terms. In comparison to the neoclassical transport coefficients, the classical coefficients are only moderately affected by a more localized $n_{z0}$, for the same reasons as discussed in relation to the amplitude scan above.

To see whether this conclusion holds for more general $n_{z0}$, we let $B_0$ in (6.1) be a non-extremum point (within the flux surface), i.e. $B_0 \in (B_{\text{min}}, B_{\text{max}})$. The resulting density distribution $n_{z0}$ will be concentrated or repelled from a contour of $B$, rather than a point, and do not necessarily represent realistic density variations: rather, they provide simple test cases very different from those considered above, and thus give an indication of how general the above conclusions are.

For $B_0 = B_{\text{min}}/2 + B_{\text{max}}/2$, the resulting $D$’s are displayed in Fig. 4. Here, the $D_{\Phi}$
increases rapidly with the amplitude, and dominates the flux except for a small interval about 0. Meanwhile, $D_T$ and $D_n$ are barely affected, with a slight reduction in magnitude when the impurities are repelled from $B_0$.

To connect this result to when $B_0$ is an extremum, we scanned $B_0$ from $B_{\text{min}}$ to $B_{\text{max}}$. The resulting $D$’s are shown in Fig. 5. Looking at $D_\Phi$, we see that as we go from $B_0 = B_{\text{min}}/2 + B_{\text{max}}/2$ ($x = 0$ in the figure) towards the extrema ($x = 1$ and $x = -1$), $D_\Phi$ tends to become less sensitive to the amplitude.

By comparing $D_\Phi$ to $D_n$ or $D_T$, in Fig. 5, we see that for all $B_0$, there are no large changes in $D_n$ or $D_T$ within the amplitude interval where $D_\Phi$ is small enough to not upset temperature screening (this interval is within or slightly outside the dashed lines, which show where $10D_\Phi = D_n + D_T$).

To conclude, it thus appears that strong $\Phi$ perturbations caused by fast particles are likely to lead to strong impurity accumulation if the radial electric field is pointing inwards, and when the $\Phi$ perturbations are weak enough so that the radial electric field
is not dominant, the condition for temperature screening is essentially unchanged from the $\Phi = 0$ case.

7. Summary & conclusions

We have derived expressions for the radial flux of high-Z collisional impurities when the bulk ions are in the $1/\nu$ regime. In this limit, the impurity temperature is equilibrated with the bulk ions, while the impurity density can vary within the flux-surface. We have derived an expression for the parallel friction-force acting on the impurities, which can be used to solve for the impurity density variations on the flux-surface, given a mechanism for relating the impurity density to the electrostatic potential.

We considered in detail the trace impurity limit, where the electrostatic potential is independent of the impurity density. Using simple models for $\Phi$ and a W7-X vacuum field, we have seen that large $\Phi$ amplitudes can cause the radial electric field to substantially contribute to the impurity transport, and lead to impurity accumulation when the radial electric field points inward. For smaller $\Phi$ amplitudes, temperature screening can be effective, and the condition for temperature screening is essentially the same as in the $\Phi = 0$ case, meaning that the temperature profile should be at least twice as steep as the density profile for screening to happen. In all cases, the contribution from classical transport is substantial, and even moderate $\Phi$ can cause the electric field to dominate if classical transport is not accounted for.

It is however not straightforward to extrapolate from these results to general $\Phi$, as the neoclassical impurity flux does not depend linearly on $n_z$, so the flux from a general $n_z$ flux-surface distribution is not a superposition of fluxes from simpler $n_z$ distributions. Realistic $\Phi$ or $n_z$ distributions may be needed to evaluate the fluxes accurately, especially when neoclassical transport is comparable to or stronger than the classical. We refer the interested reader to Calvo et al. (2018), where an LHD equilibrium with a $\Phi$ set up by particle trapping effects of the bulk ions is considered.

The authors are grateful for the fruitful discussions with the authors of Calvo et al. (2018), who considered the same problem independently and in parallel to us, from which we have benefited. This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission. SB and IP were supported by the International Career Grant of Vetenskapsrådet (Dnr. 330-2014-
Appendix A. Solving the ion drift-kinetic equation

In this section, we solve (3.7) for \( F^{(0)}_{i1} \). The solution follows \cite{Newton2017}, but here \( n_z \) is allowed to vary on the flux-surface. Since we assume \( e\Phi/T_i \sim Z^{-1} \), the potential energy of the bulk ions is approximately constant on the flux-surface, and we change variables from \( E, \mu \) to the approximate invariants \( v, \lambda \).

Equation 3.7 can be formally solved by integrating along a field-line; using \( l \) to denote the distance along the field line, we have

\[
F^{(0)}_{i1}(l) = F^{(0)}_{i1}(l_0) - \int_{l_0}^{l} \frac{dl'}{v_{\parallel}} v_d \cdot \nabla f_{i0}(l'),
\]

(A 1)

where \( l_0 \) is an arbitrary point along the field line and the integration constant \( F^{(0)}_{i1}(l_0) \) is set by the solvability condition of the first-order equation. As only the parts of \( F^{(0)}_{i1}(l_0) \) that are odd in \( v_{\parallel} \) will contribute to the parallel friction force, it is convenient to take \( l_0 \) as a bounce-point, \( B(l_0) = 1/\lambda \), which sets the odd part of \( F^{(0)}_{i1}(l_0) \) to zero in the trapped region.

In the passing region, \( F^{(0)}_{i1} \) is set by

\[
\left< \frac{B}{v_{\parallel}} C_i[F^{(0)}_{i1}] \right> = 0.
\]

(A 2)

Using \( \mathcal{L} = \frac{2v_{\parallel}^2}{eB} \frac{\partial}{\partial \lambda} \lambda v_{\parallel} \frac{\partial}{\partial \lambda} \), and integrating once with respect to \( \lambda \), (A 2) becomes

\[
\frac{\partial}{\partial \lambda} F^{(0)}_{i1}(l_0) = - \frac{mv_{\parallel}^2}{2 \left< \frac{[1 + \frac{\nu_{i1}^D(l)}{v_{\parallel}^D}]}{v_{\parallel}} \right>} \left( \frac{1}{e} \left[ \left[ 1 + \frac{\nu_{i1}^D(l)}{v_{\parallel}^D} \right] g_4(l, \lambda) \right] \frac{\partial f_{i0}}{\partial \psi} + \frac{1}{T_i} f_{i0} \left< B \left[ U_{\parallel} + \frac{\nu_{i1}^D(l)}{v_{\parallel}^D} V_{\parallel} \right] \right> \right)
\]

in the passing region. To account for the \( v_d \cdot \nabla f_{i0} \) term, we have introduced the geometric function \cite{Nakajima1989}

\[
g_4(\lambda, l) = v_{\parallel} \int_{l_0}^{l} dl' (b \times \nabla \psi) \cdot \nabla \left( \frac{1}{v_{\parallel}} \right).
\]

(A 4)

Appendix B. Parallel friction force

Once \( U_{\parallel} \) and \( V_{\parallel} \) are known, we can use (A 3) to directly evaluate the parallel friction force acting on the impurities. From our mass-ratio expanded ion-impurity collision operator (3.2) and the self-adjointness of the Lorentz operator, we have

\[
R_{iz_{\parallel}} = \int d^3v m_i v_{\parallel} v_{\parallel}^D(v) \left( \frac{m_i v_{\parallel} \cdot V_{\parallel}}{T_i} f_{i0} - F_{i1} \right)
\]

\[
= \frac{n_i m_i}{\tau_{iz}} \left( V_{\parallel} - \frac{T_i}{e} \left[ A_{i1} - \frac{3}{2} A_{i2} \right] Bu - BP(\psi) \right),
\]

(B 1)
where $P$ is a flux-function which contains the contribution from the integration constant $F_{i1}^{(0)}(l_0)\) 

$$P(\psi) = \frac{\tau_{iz}}{Bn_i} \int d^3v v || v_D^{iiz} F_{i1}^{(0)}(l_0).$$  \tag{B2}$$
P(\psi) can be evaluated using \(A3\) and partial integration in $\lambda$

$$P(\psi) = \frac{\langle BU \rangle}{\langle B^2 \rangle} b_1 + \frac{\langle \alpha BV z \rangle}{\langle B^2 \rangle} b_4 + \frac{T_i}{e} \left[ A_{1i} - \frac{5}{2} A_{2i} \right] b_2 + \frac{T_i}{e} \frac{A_{2i}}{\langle B^2 \rangle} b_3 \tag{B3}$$

where we have introduced

$$b_1 = \frac{m\pi \langle B^2 \rangle}{n_i T_i \langle \nu_D^{iiz} \rangle} \int_0^\infty dv v^4 \nu_D^{iiz} f_i \int_0^{1/B_{max}} d\lambda \frac{1}{\langle \xi \rangle + \langle \nu_D^{iiz} \xi \rangle} \tag{B4}$$

$$b_2 = \frac{m\pi \langle B^2 \rangle}{n_i T_i \langle \nu_D^{iiz} \rangle} \int_0^\infty dv v^4 \nu_D^{iiz} f_i \int_0^{1/B_{max}} d\lambda \frac{\langle g_4 \rangle + \langle \nu_D^{iiz} g_4 \rangle}{\langle \xi \rangle + \langle \nu_D^{iiz} \xi \rangle} \tag{B5}$$

$$b_3 = \frac{m\pi \langle B^2 \rangle}{n_i T_i \langle \nu_D^{iiz} \rangle} \int_0^\infty dv v^4 \frac{m_i v^2}{2T_i} \nu_D^{iiz} f_i \int_0^{1/B_{max}} d\lambda \frac{\langle g_4 \rangle + \langle \nu_D^{iiz} g_4 \rangle}{\langle \xi \rangle + \langle \nu_D^{iiz} \xi \rangle} \tag{B6}$$

$$b_4 = \frac{m\pi \langle B^2 \rangle}{Z^2 n_i T_i \langle \nu_D^{iiz} \rangle} \int_0^\infty dv v^4 \nu_D^{iiz} f_i \int_0^{1/B_{max}} d\lambda \frac{1}{\langle \xi \rangle + \langle \nu_D^{iiz} \xi \rangle}, \tag{B7}$$

with $\xi = v \cdot b/v$. The velocity average $\{ \cdot \}$ is defined as

$$\{F(v)\} \equiv \frac{8}{3\sqrt{\pi}} \int_0^\infty dx F(x)x^4 e^{-x^2}, \tag{B8}$$

where $x = v/v_{Ti}$.

To have the boundary terms from the partial integration disappear in \(B3\), we have defined $l_0$ through $B(l_0) = B_{max}$. This makes our choice of $l_0$ continuous when going from the trapped to the passing region, and thus ensures that $F_{i1}^{(0)}(l_0)$ is zero at the trapped-passing boundary $\lambda = 1/B_{max}$.

### Appendix C. Momentum restoring term $U_{||}$

The momentum restoring term in the ion-ion model collision operator \(3.5\) is calculated so that ion-ion collisions conserve momentum. Specifically, we have

$$U_{||} = \frac{1}{n_i \langle \nu_D^{iiz} \rangle} \int d^3v v || v_D^{iiz} F_{i1}^{(0)}. \tag{C1}$$

Inserting $F_{i1}^{(0)}$ from \(A1\) and using \(A3\), we get

$$\langle BU \rangle (1 - a_1) = \frac{T_i}{e} \left[ \langle a_2 + \langle uB^2 \rangle \rangle A_{1i} + \left[ a_3 - \frac{5}{2} a_2 - \langle uB^2 \rangle \eta \right] A_{2i} \right] + a_4 \langle \alpha BV z \rangle.$$

\(C2\)
where we have defined the geometry-impurity dependent flux-surface constants

\[
a_1 = \frac{m\pi \langle B^2 \rangle}{n_i T_i \{\nu_D^i\}} \int_0^\infty dv v^4 \nu_D^i f_{i0} \int_0^{1/B_{\text{max}}} d\lambda \frac{1}{\langle \xi \rangle + \langle \nu_D^i \nu_D^i \rangle} \]  
\hspace{1cm} (C3)

\[
a_2 = \frac{m\pi \langle B^2 \rangle}{n_i T_i \{\nu_D^i\}} \int_0^\infty dv v^4 \nu_D^i f_{i0} \int_0^{1/B_{\text{max}}} d\lambda \frac{\langle g_4 \rangle + \langle \nu_D^i \nu_D^i g_4 \rangle}{\langle \xi \rangle + \langle \nu_D^i \nu_D^i \rangle} \]  
\hspace{1cm} (C4)

\[
a_3 = \frac{m\pi \langle B^2 \rangle}{n_i T_i \{\nu_D^i\}} \int_0^\infty dv v^4 m_i v^2 \nu_D^i f_{i0} \int_0^{1/B_{\text{max}}} d\lambda \frac{\langle g_4 \rangle + \langle \nu_D^i \nu_D^i g_4 \rangle}{\langle \xi \rangle + \langle \nu_D^i \nu_D^i \rangle} \]  
\hspace{1cm} (C5)

\[
a_4 = \frac{m\pi \langle B^2 \rangle}{Z^2 n_z T_i \{\nu_D^i\}} \int_0^\infty dv v^4 \nu_D^z f_{z0} \int_0^{1/B_{\text{max}}} d\lambda \frac{1}{\langle \xi \rangle + \langle \nu_D^i \nu_D^i \rangle} \]  
\hspace{1cm} (C6)

and the boundary condition for \( u \) is \( u(l_0) = 0 \).

**Appendix D. Solvability condition and \( K_z \)**

From (2.15), \( V_{z||} \) is known up to a flux-function \( K_z \). The solvability condition of (2.2) states that

\[
\frac{\langle BR_{z||} \rangle}{n_z} = 0,
\]  
\hspace{1cm} (D1)

which we use to determine \( K_z \). Inserting (B1), the solvability condition becomes

\[
\frac{n_i m_i}{n_z \tau_{iz}} \left( \langle BV_{z||} \rangle - \frac{T_i}{e} \left[ A_{i1} - \frac{3}{2} A_{i2} \right] \langle uB^2 \rangle - \langle B^2 \rangle P(\psi) \right) = 0.
\]  
\hspace{1cm} (D2)

For the sake of compactness, we also define

\[
c_1 = b_1/(1 - a_1), \]  
\hspace{1cm} (D3)

\[
c_4 = b_4 + a_4 c_1; \]  
\hspace{1cm} (D4)

this results in (3.10).

**Appendix E. Trace impurity limit of some expressions**

In the trace impurity limit, \( \alpha \equiv Z^2 n_z/n_i \ll 1 \), the \( a_i, b_j \) and \( c_k \)'s simplify considerably, yielding an expression for \( K_z \) in terms of standard geometry functions. Specifically,

\[
a_1 = b_1 = f_c, \]  
\hspace{1cm} (E1)

\[
a_2 = b_2 = f_s, \]  
\hspace{1cm} (E2)

\[
a_3 = f_s \left( \frac{5}{2} - \eta \right), \]  
\hspace{1cm} (E3)

\[
b_3 = f_s, \]  
\hspace{1cm} (E4)

\[
a_4 = \frac{f_c \nu_D^i}{\alpha \nu_D^i}, \]  
\hspace{1cm} (E5)

\[
b_4 = \frac{f_c \nu_D^z}{\alpha \nu_D^i}. \]  
\hspace{1cm} (E6)
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Note that $a_4$ and $b_4$ only appear in terms containing $\alpha$, which are negligible in the trace-limit. Here,

$$f_c = \frac{3}{4} \langle B^2 \rangle \int_0^{1/B_{\max}} d\lambda \lambda \langle \xi \rangle$$

(E7)

$$f_s = \frac{3}{4} \langle B^2 \rangle \int_0^{1/B_{\max}} d\lambda \lambda \langle g_4 \rangle$$

(E8)

are standard functions of geometry. With this, $K_z$ becomes

$$K_z(\psi) \left\langle \frac{B^2}{n_z} \right\rangle = \frac{T_i}{e} \left[ f_s + \langle uB^2 \rangle \right] \left( \left[ \frac{f_c}{1 - f_c} + 1 \right] A_{1i} - \left[ \frac{nf_c}{1 - f_c} + \frac{3}{2} \right] A_{2i} \right) - \frac{d \langle \Phi \rangle}{d\psi} \langle uB^2 \rangle. \quad (E9)$$

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