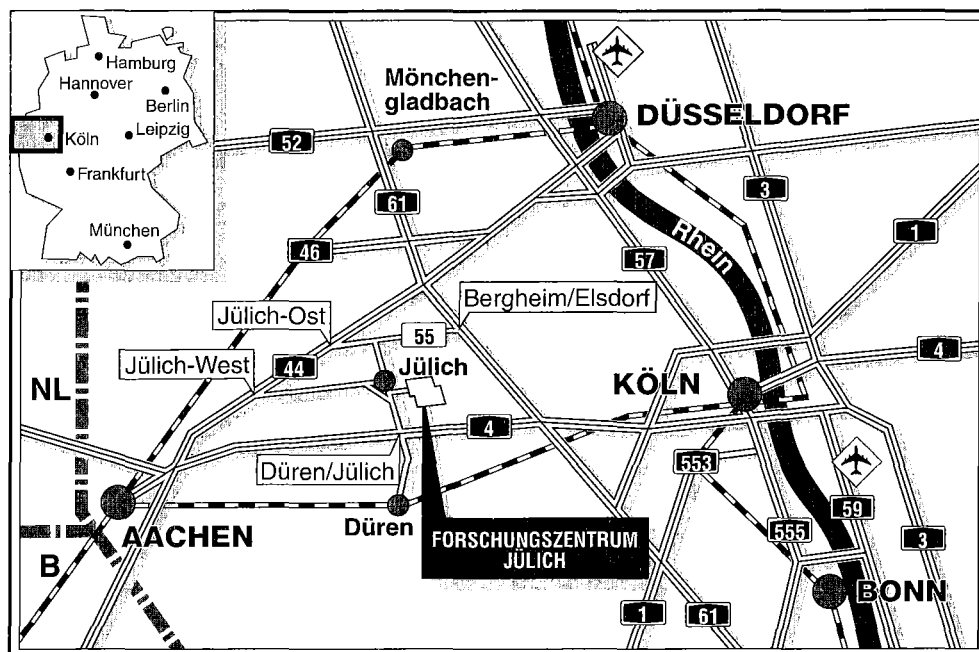


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Calculation of $\parallel \vec{B}$ Transport Coefficients and the
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Berichte des Forschungszentrums Jülich ; 3287

ISSN 0944-2952

Institut für Plasmaphysik Jül-3287

Association EURATOM-KFA

Zu beziehen durch: Forschungszentrum Jülich GmbH · Zentralbibliothek
D-52425 Jülich · Bundesrepublik Deutschland

Telefon: 02461/61-61 02 · Telefax: 02461/61-61 03 · Telex: 833 556-70 kfa d

The Method of Reduced Charge States for the Calculation of $\parallel \vec{B}$ Transport Coefficients and the Neoclassical Particle and Heat Fluxes

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Abstract:

The paper briefly summarizes the method of reduced charge states, which is an almost exact method and serves to reduce the number of equations, which have to be solved simultaneously in the calculation of particle and heat fluxes. The method can be applied to both longitudinal ($\parallel \vec{B}$) and cross-field ($\perp \vec{B}$) transport theory and becomes increasingly important with the number of plasma ion species under consideration. In the present report we deal only with the longitudinal and the attributed neoclassical radial transport in toroidal magnetized plasmas. The calculations are performed within Grad's 21-moment approximation for the distribution functions of the various charge carriers. They are restricted to the collision-dominated (Pfirsch-Schlüter) transport regime. The method of derivation is outlined, and the results are compared with existing formulations, showing that earlier incomplete or incorrect formulae have to be revised. Only the most recent results [6] corresponding to Grad's 13-moment approximation agree with ours in the same approximation. Although for sake of clarity the calculations have been performed in the standard magnetic field geometry with concentric circular magnetic flux surfaces, they could be readily generalized for arbitrary magnetic field configurations.

I. Charge averaging of $\|\vec{B}\|$ fluxes in the 21-moment approximation

The starting point of the present study is the system of (collision-dominated) transport equations for the charge averaged values of the longitudinal ($\|\vec{B}\|$) diffusive mass and heat fluxes $\rho_\alpha \bar{w}_{\alpha\|}$, $\bar{h}_{\alpha\|}$ and $\bar{r}_{\alpha\|}$ appearing in the 21-moment approximation (with $R_{\alpha\|} = \sum_z R_{\alpha z\|}$, $H_{\alpha\|} = \sum_z H_{\alpha z\|}$ and $\rho_\alpha = \sum_z \rho_{\alpha z} \equiv m_\alpha \sum_z n_{\alpha z}$) as outlined in ref.[1] (for the principles of the method see also ref.[2])

$$F_a = \sum_b c_{ab} W_b, \quad \text{where} \quad F_a = \begin{pmatrix} -K_{\alpha\|}/\rho_\alpha \\ -\nabla_{\|} \ln T \\ 0 \end{pmatrix}, \quad W_b = \begin{pmatrix} \rho_\beta \bar{w}_{\beta\|} \\ \bar{h}_{\beta\|} \\ \bar{r}_{\beta\|} \end{pmatrix}$$

are vectors of $3N$ elements with $\alpha, \beta = 1, 2, \dots, N$ denoting the number of ion species (different elements) in the plasma. The above set of equations, which couples conjugate thermodynamic fluxes and forces, is derived from

$$K_{\alpha\|} \equiv \nabla_{\|} p_\alpha - n_\alpha \bar{z}_\alpha e E_{\|} + \rho_\alpha \left(\frac{d\vec{U}}{dt} \right)_{\|} = R_{\alpha\|} \equiv \sum_z \int m_\alpha c_{\alpha z\|} \frac{\partial_s f_{\alpha z}}{\partial t} d^3 c_{\alpha z}$$

$$\text{and} \quad \frac{5}{2} \frac{p_\alpha}{m_\alpha} \nabla_{\|} (kT) = H_{\alpha\|} \equiv \sum_z \int \left(\frac{m_\alpha}{2} c_{\alpha z}^2 - \frac{5}{2} kT \right) c_{\alpha z\|} \frac{\partial_s f_{\alpha z}}{\partial t} d^3 c_{\alpha z}$$

$$\text{where} \quad \vec{U} \equiv \frac{\sum_\alpha \sum_z \rho_{\alpha z} \vec{U}_{\alpha z}}{\sum_\alpha \rho_\alpha} \quad \text{and} \quad \vec{c}_{\alpha z} = \vec{v}_{\alpha z} - \vec{U}$$

are respectively the center-of-mass velocity of the ensemble of all ion species, which is nearly equal to the center-of-mass velocity of the whole plasma, and the relative velocity of an individual particle with respect to the center-of-mass velocity. $R_{\alpha\|}$ and $H_{\alpha\|}$ denote the $\|\vec{B}\|$ components of the collisional mass respectively heat transfer from the considered species α to any species β ($\partial_s f_\alpha / \partial t$ being the collision term in the kinetic equation). The first one is the conventional resistive force, the second one describes the flow of resistive heating power. Note that here and in all formulae to follow the

charge averaged quantities

$$\bar{z}_\alpha^k \equiv \frac{\sum_z z^k n_{\alpha z}}{n_\alpha} \quad \text{and} \quad \begin{pmatrix} \rho_\alpha \bar{w}_{\alpha||} \\ \bar{h}_{\alpha||} \\ \bar{r}_{\alpha||} \end{pmatrix} \equiv \sum_z \frac{z^2}{\bar{z}_\alpha^2} \begin{pmatrix} \rho_{\alpha z} w_{\alpha z||} \\ h_{\alpha z||} \\ r_{\alpha z||} \end{pmatrix}$$

are used ($\bar{z}_\alpha \equiv \bar{z}_\alpha^1$), where the fluxes are defined by

$$\rho_{\alpha z} w_{\alpha z||} = m_\alpha \int c_{\alpha z||} f_{\alpha z} d^3 c_{\alpha z}$$

$$h_{\alpha z||} = q_{\alpha z||} - \frac{5}{4} v_{T\alpha}^2 \rho_{\alpha z} w_{\alpha z||} \quad \text{with} \quad q_{\alpha z||} = \frac{m_\alpha}{2} \int c_{\alpha z}^2 c_{\alpha z||} f_{\alpha z} d^3 c_{\alpha z}$$

$$r_{\alpha z||} = \frac{m_\alpha}{4} \int \left(c_{\alpha z}^4 - 7 v_{T\alpha}^2 c_{\alpha z}^2 + \frac{35}{4} v_{T\alpha}^4 \right) c_{\alpha z||} f_{\alpha z} d^3 c_{\alpha z}$$

$$= \frac{m_\alpha}{4} \int c_{\alpha z}^4 c_{\alpha z||} f_{\alpha z} d^3 c_{\alpha z} - \frac{7}{2} v_{T\alpha}^2 q_{\alpha z||} + \frac{35}{16} v_{T\alpha}^4 \rho_{\alpha z} w_{\alpha z||} \quad \text{with} \quad v_{T\alpha}^2 = \frac{2kT}{m_\alpha}$$

The above definition of charge averaged quantities is, strictly speaking, only meaningful, if we ignore the charge state dependence of the Coulomb logarithm (see below). The error introduced by this approximation is, however, small. Also note that in a spatially inhomogeneous magnetic field curvature and mirror effects appear and therefore $(d\vec{U}/dt)_|| \neq dU_||/dt$. In the above form the expressions for the charge averaged fluxes are only valid in case of a common ion temperature (i.e. strong temperature equilibration) such that $p_\alpha = n_\alpha kT$. The matrix c_{ab} containing $9N^2$ elements is defined by

$$c_{ab} = \begin{pmatrix} c_{\alpha\beta}^{(11)} & c_{\alpha\beta}^{(12)} & c_{\alpha\beta}^{(13)} \\ c_{\alpha\beta}^{(21)} & c_{\alpha\beta}^{(22)} & c_{\alpha\beta}^{(23)} \\ c_{\alpha\beta}^{(31)} & c_{\alpha\beta}^{(32)} & c_{\alpha\beta}^{(33)} \end{pmatrix}$$

with the 9 submatrices each containing N^2 elements (see ref.[1])

$$\begin{aligned}
c_{\alpha\beta}^{(11)} &= \frac{\bar{G}_{\alpha\beta}^{(1)} - \delta_{\alpha\beta} \sum_{\kappa} \bar{G}_{\alpha\kappa}^{(1)}}{\rho_{\alpha}\rho_{\beta}} \quad ; \quad c_{\alpha\beta}^{(12)} = \frac{\mu_{\alpha\beta}\bar{G}_{\alpha\beta}^{(2)} - \delta_{\alpha\beta} \sum_{\kappa} \mu_{\alpha\kappa}\bar{G}_{\alpha\kappa}^{(2)}}{\rho_{\alpha}\rho_{\beta} kT} = c_{\alpha\beta}^{(21)} \\
c_{\alpha\beta}^{(13)} &= \frac{\mu_{\alpha\beta}^2 \bar{G}_{\alpha\beta}^{(3)} - \delta_{\alpha\beta} \sum_{\kappa} \mu_{\alpha\kappa}^2 \bar{G}_{\alpha\kappa}^{(3)}}{\rho_{\alpha}\rho_{\beta} (kT)^2} = c_{\alpha\beta}^{(31)} \quad ; \quad c_{\alpha\beta}^{(22)} = \frac{2}{5} \frac{\bar{G}_{\alpha\beta}^{(5)} - \delta_{\alpha\beta} \sum_{\kappa} \bar{G}_{\alpha\kappa}^{(4)}}{p_{\alpha}p_{\beta}} \\
c_{\alpha\beta}^{(23)} &= \frac{2}{5} \frac{\mu_{\alpha\beta}\bar{G}_{\alpha\beta}^{(7)} - \delta_{\alpha\beta} \sum_{\kappa} \mu_{\alpha\kappa}\bar{G}_{\alpha\kappa}^{(6)}}{p_{\alpha}p_{\beta} kT} = c_{\alpha\beta}^{(32)} \\
c_{\alpha\beta}^{(33)} &= \frac{2}{35} \frac{m_{\alpha}m_{\beta}(\bar{G}_{\alpha\beta}^{(9)} - \delta_{\alpha\beta} \sum_{\kappa} \bar{G}_{\alpha\kappa}^{(8)})}{p_{\alpha}p_{\beta}(kT)^2}
\end{aligned}$$

where $\mu_{\alpha\beta} = m_{\alpha}m_{\beta}/(m_{\alpha} + m_{\beta})$ is the reduced mass and $\delta_{\alpha\beta}$ is the Kronecker symbol to denote the unit matrix. The coefficients $c_{\alpha\beta}^{(3k)}$ with $k = 1, 2, 3$ follow from multiplication of equ.(2c), ref.[1] by $-16/(35v_T^6 p_{\alpha})$. Note that the matrix elements are completely symmetric in the upper indices and therewith satisfy the Onsager relations.

According to Cramer's rule the formal solution (inversion) of the above linear vector equation reads ($|\dots|$ denoting determinants)

$$W_b = \frac{|F_a \delta_{kb} + c_{ak}(1 - \delta_{kb})|}{|c_{ak}|}$$

In order to get an explicit representation of the thermodynamic fluxes W_b in terms of the thermodynamic forces F_a , one should expand the determinant in the numerator of this expression in the elements F_a of column b. In the above mentioned approximation $\ln \Lambda_{\alpha z, \beta \zeta} \simeq \ln \Lambda$ for the Coulomb logarithm we get

$$\bar{G}_{\alpha\beta}^{(n)} \equiv \sum_{z, \zeta} G_{\alpha z, \beta \zeta}^{(n)} = Q_+^* g_{\alpha\beta}^{(n)} \sqrt{\mu_{\alpha\beta}} n_{\alpha} n_{\beta} \bar{z}_{\alpha}^2 \bar{z}_{\beta}^2$$

introducing the quantity (compare ref.[3], p.9)

$$Q_+^* = \frac{4\sqrt{2\pi}}{3} \left(\frac{e^2}{4\pi\epsilon_0} \right)^2 \frac{\ln \Lambda}{\sqrt{kT^3}}$$

and the functions $g_{\alpha\beta}^{(n)} = g^{(n)}(m_\alpha/m_\beta)$ as given in the Appendix. Then the relation $c_{ab} = Q_+^* c_{ab}^*$ holds such that (compare ref.[3], p.11)

$$W_b = \frac{|F_a \delta_{kb} + c_{ak}^* (1 - \delta_{kb})|}{Q_+^* |c_{ak}^*|}$$

Once the solution for the charge averaged fluxes W_b has been found, the individual fluxes can be derived by a set of equations, which only contain the thermodynamic forces of the ion species under consideration. In particular

$$w_{\alpha z||} = \bar{w}_{\alpha||} + \frac{1}{\kappa_\alpha^{(1)}} \left(\frac{n_\alpha \bar{z}_\alpha^2 R_{\alpha z||}}{z^2 n_{\alpha z}} - R_{\alpha||} \right) - \frac{\kappa_\alpha^{(4)}}{\kappa_\alpha^{(1)}} n_\alpha \left(\frac{\bar{z}_\alpha^2}{z^2} - 1 \right) \nabla_{||}(kT)$$

$$\frac{h_{\alpha z||}}{p_{\alpha z}} = \frac{\bar{h}_{\alpha||}}{p_\alpha} + \frac{\kappa_\alpha^{(4)}}{\kappa_\alpha^{(1)}} \left(\frac{n_\alpha \bar{z}_\alpha^2 R_{\alpha z||}}{z^2 n_{\alpha z}} - R_{\alpha||} \right) + \frac{\kappa_\alpha^{(3)}}{\kappa_\alpha^{(1)}} n_\alpha \left(\frac{\bar{z}_\alpha^2}{z^2} - 1 \right) \nabla_{||}(kT)$$

$$\frac{r_{\alpha z||}}{p_{\alpha z}} = \frac{\bar{r}_{\alpha||}}{p_\alpha} - \frac{kT}{m_\alpha S_\alpha^{(8)}} \left[S_\alpha^{(3)} (w_{\alpha z||} - \bar{w}_{\alpha||}) + 7 S_\alpha^{(6)} \left(\frac{h_{\alpha z||}}{p_{\alpha z}} - \frac{\bar{h}_{\alpha||}}{p_\alpha} \right) \right]$$

where we have introduced the coefficients

$$\kappa_\alpha^{(1)} = \kappa_\alpha^{(2)} + \frac{(2/5)}{S_\alpha^{(8)}} \frac{\left(S_\alpha^{(2)} S_\alpha^{(8)} - S_\alpha^{(3)} S_\alpha^{(6)} \right)^2}{S_\alpha^{(4)} S_\alpha^{(8)} - 7[S_\alpha^{(6)}]^2} \quad \text{with} \quad \kappa_\alpha^{(2)} = S_\alpha^{(1)} - \frac{2}{35} \frac{[S_\alpha^{(3)}]^2}{S_\alpha^{(8)}}$$

$$\kappa_\alpha^{(3)} = \frac{(5/2) \kappa_\alpha^{(2)} S_\alpha^{(8)}}{S_\alpha^{(4)} S_\alpha^{(8)} - 7[S_\alpha^{(6)}]^2} \quad ; \quad \kappa_\alpha^{(4)} = \frac{S_\alpha^{(2)} S_\alpha^{(8)} - S_\alpha^{(3)} S_\alpha^{(6)}}{S_\alpha^{(4)} S_\alpha^{(8)} - 7[S_\alpha^{(6)}]^2}$$

using the coefficients $S_\alpha^{(k)}$ and $\kappa_\alpha^{(4)} \equiv c_\alpha^{(6)}$ from ref.[1] (see Appendix). We recall that

$$\frac{n_\alpha \bar{z}_\alpha^2 R_{\alpha z}}{z^2 n_{\alpha z}} - R_{\alpha \parallel} =$$

$$\left(\frac{n_\alpha \bar{z}_\alpha^2 \nabla_{\parallel} p_{\alpha z}}{z^2 n_{\alpha z}} - \nabla_{\parallel} p_\alpha \right) - \left(\frac{\bar{z}_\alpha^2}{z^2} - \frac{\bar{z}_\alpha}{z} \right) n_\alpha z e E_{\parallel} + \left(\frac{\bar{z}_\alpha^2}{z^2} - 1 \right) m_\alpha n_\alpha \left(\frac{d\vec{U}}{dt} \right)_{\parallel}$$

The charge averaged fluxes have to be distinguished from the total fluxes:

$$\Gamma_{\alpha \parallel} \equiv \sum_z n_{\alpha z} (w_{\alpha z \parallel} + U_{\parallel}) =$$

$$\frac{n_\alpha}{\kappa_\alpha^{(1)}} \left[\left(\sum_z \frac{\bar{z}_\alpha^2 \nabla_{\parallel} p_{\alpha z}}{z^2} - \nabla_{\parallel} p_\alpha \right) - \left(\sum_z \frac{\bar{z}_\alpha^2 n_{\alpha z}}{z} - \bar{z}_\alpha n_\alpha \right) e E_{\parallel} \right] +$$

$$+ \frac{n_\alpha}{\kappa_\alpha^{(1)}} \left(\sum_z \frac{\bar{z}_\alpha^2 n_{\alpha z}}{z^2} - n_\alpha \right) \left[m_\alpha \left(\frac{d\vec{U}}{dt} \right)_{\parallel} - \kappa_\alpha^{(4)} \nabla_{\parallel} (kT) \right] + n_\alpha (\bar{w}_{\alpha \parallel} + U_{\parallel})$$

$$h_{\alpha \parallel} \equiv \sum_z h_{\alpha z \parallel} = \frac{p_\alpha \kappa_\alpha^{(4)}}{\kappa_\alpha^{(1)}} \left[\left(\sum_z \frac{\bar{z}_\alpha^2 \nabla_{\parallel} p_{\alpha z}}{z^2} - \nabla_{\parallel} p_\alpha \right) - \left(\sum_z \frac{\bar{z}_\alpha^2 n_{\alpha z}}{z} - \bar{z}_\alpha n_\alpha \right) e E_{\parallel} \right] +$$

$$+ \frac{p_\alpha}{\kappa_\alpha^{(1)}} \left(\sum_z \frac{\bar{z}_\alpha^2 n_{\alpha z}}{z^2} - n_\alpha \right) \left[\kappa_\alpha^{(4)} m_\alpha \left(\frac{d\vec{U}}{dt} \right)_{\parallel} + \kappa_\alpha^{(3)} \nabla_{\parallel} (kT) \right] + \bar{h}_{\alpha \parallel}$$

These equations can only be exploited in connection with the particle balance equations for the individual charge states of the ion species α . It appears that the differences between total and charge-averaged fluxes also contain terms $\sim \bar{z}_\alpha^k$ with $k = -1, -2$. Note that in fusion plasmas the population densities of the different charge states of low-Z impurities cannot be described by the Corona model due to the comparable strength of inelastic collisions and cross-field transport processes, which are governed by both anomalous and neoclassical effects. Since $q^2 \gg 1$ (q =safety factor), the latter are predominantly related to the classical transport along the magnetic field under consideration here.

II. Radial neoclassical fluxes resulting from $\|\vec{B}$ friction forces

To illustrate the way, in which the method of reduced charge states enters the derivation of the neoclassical fluxes perpendicular to the magnetic flux surfaces of an axisymmetric toroidal system we adopt a toroidal coordinate system (r, θ, ϕ) with $\partial/\partial\phi = 0$ and the standard magnetic field configuration $\vec{B} = (0, -\Theta, 1)B_\phi$ with $\Theta = -B_\theta/B_\phi = \Theta(r) > 0$, $B_\phi R = \text{const.}$ and $R = R_0 + r \cos \theta$ leading to circular concentric magnetic flux surfaces as given in fig.1. The physics and couplings (indicating the calculation procedure) underlying the neoclassical transport are shown in fig.2 and fig.3. In the standard magnetic field geometry the neoclassical contributions to the radial particle and heat fluxes, which are related to the collisional particle and heat transport $\|\vec{B}$ by the toroidal momentum and heat flux balance, read (neglecting the term $\sim (d\vec{U}/dt)_\parallel$)

$$\Gamma_{\alpha z, r} = \frac{R_{\alpha z \parallel}}{m_\alpha \Theta \Omega_{\alpha z}} \quad \text{and} \quad h_{\alpha z, r} = \frac{H_{\alpha z \parallel}}{\Theta \Omega_{\alpha z}}$$

where $\Omega_{\alpha z} \equiv zeB/m_\alpha$. The corresponding magnetic flux surface averages are defined by

$$\langle \Gamma_{\alpha z, r}, h_{\alpha z, r} \rangle \equiv \oint \frac{d\theta}{2\pi} \frac{R}{R_0} (\Gamma_{\alpha z, r}, h_{\alpha z, r}) = \oint \frac{d\theta}{2\pi} \frac{R/R_0}{\Theta \Omega_{\alpha z}} \left(\frac{R_{\alpha z \parallel}}{m_\alpha}, H_{\alpha z \parallel} \right)$$

In the following we show the calculation method in some detail for the neoclassical particle flux (the heat flux calculations proceed analogously) and first consider the contribution arising from the friction force in the $\|\vec{B}$ momentum equation of the element α in charge state z :

$$R_{\alpha z \parallel}^U = \sum_{\beta} I_{\alpha z} \bar{G}_{\alpha\beta}^{(1)} \left(\frac{\Gamma_{\alpha z \parallel}}{n_{\alpha z}} - \frac{\bar{\Gamma}_{\beta \parallel}}{n_{\beta}} \right) \quad ; \quad I_{\alpha z} \equiv \frac{z^2 n_{\alpha z}}{z_\alpha^2 n_\alpha}$$

To average $\Gamma_{\alpha z, r}$ over a magnetic surface, we need the poloidal dependence of $\Gamma_{\alpha z \parallel}$ as resulting from the particle balance equation (see ref.[4],p.17)

$$-\frac{\Theta}{rR} \frac{\partial(R\Gamma_{\alpha z\parallel})}{\partial\theta} = -\nabla_v \Gamma_{\alpha z,v}^{nc} + \frac{2n_{\alpha z} \nabla_v \Phi}{BR} +$$

$$+ \frac{(\vec{\nabla} n_{\alpha z} \times \vec{\nabla} \Phi)_\phi}{B} + \frac{1}{rR} \frac{\partial}{\partial r} \left(rR D_{\alpha z\perp} \frac{\partial n_{\alpha z}}{\partial r} \right) + \delta S_{\alpha z}$$

$$\text{where } -\Gamma_{\alpha z,v}^{nc} \equiv 2\pi \int_0^{+\infty} dv_\perp v_\perp \int_{-\infty}^{+\infty} dv_\parallel \frac{v_\parallel^2 + v_\perp^2/2}{\Omega_{\alpha z} R} F_{\alpha z}(\vec{x}, v_\parallel, v_\perp)$$

$$\Rightarrow \frac{2p_{\alpha z}}{m_\alpha \Omega_{\alpha z} R} \left(1 + \frac{U_\parallel^2}{v_{T\alpha}^2} \right)$$

$$\text{for } F_{\alpha z}(\vec{x}, v_\parallel, v_\perp) = \frac{n_{\alpha z}}{(\sqrt{\pi} v_{T\alpha})^3} \exp \left[-\frac{(v_\parallel - U_\parallel)^2 + v_\perp^2}{v_{T\alpha}^2} \right]$$

i.e. for a local shifted Maxwellian distribution function related to the mean mass velocity $U_\parallel$ of the plasma mixture (as the leading term in Grad's expansion in irreducible Hermite polynomials) assuming, as before, temperature isotropy with a common temperature for all ion species (i.e. considering the strong temperature equilibration case). Note that in this representation pressure and temperature are defined in a coordinate system moving with $U_\parallel$ instead of $U_{\alpha z\parallel}$. $D_{\alpha z\perp}$, $\delta S_{\alpha z}$, and ∇_v denote respectively the coefficient for anomalous diffusion in radial direction, the effective particle source and the derivative with respect to the vertical coordinate as defined by

$$\nabla_v \equiv \cos \theta \frac{\partial}{r \partial \theta} + \sin \theta \frac{\partial}{\partial r}$$

Note that the vertical particle and (see below) heat drift fluxes have a negative sign in the adopted coordinate system (fig.1), where the vertical axis points upwards.

We consider the first two terms on the rhs of the particle balance equation to be the dominant ones (neglecting anomalous transport and source terms, for a more complete treatment including inelastic collision processes see

ref.[4]) and assume both $U_{\parallel}^2/v_{T\alpha}^2 \ll 1$ and $r/R_0 \ll 1$ (plasma column with large aspect ratio). In this approximation the contribution $\sim \cos \theta (\partial/r \partial \theta)$ to ∇_v is also neglected with the result that

$$\Gamma_{\alpha z \parallel} \simeq \frac{2r \cos \theta}{m_{\alpha} \Omega_{\alpha z} \Theta R} \left(\frac{\partial p_{\alpha z}}{\partial r} + z e n_{\alpha z} \frac{\partial \Phi}{\partial r} \right)$$

Inserting the above expression via $R_{\alpha z \parallel}$ into the equation for $\Gamma_{\alpha z, r}$ and taking into account that $g^{(1)}(m_{\alpha}/m_{\beta}) = -1$ (see p.3) we obtain

$$\Gamma_{\alpha z, r}^U \simeq - \frac{2r \cos \theta Q_+^* p_{\alpha z}}{(eB\Theta)^2 R} \sum_{\beta} \sqrt{\mu_{\alpha\beta}} n_{\beta} \left[\bar{z}_{\beta}^2 \frac{\partial \ln p_{\alpha z}}{\partial r} - z \bar{z}_{\beta} \frac{\partial \ln(\bar{z}_{\beta} p_{\beta})}{\partial r} \right]$$

and, introducing the safety factor $q \equiv r/(\Theta R_0)$, the averaged value

$$\langle \Gamma_{\alpha z, r}^U \rangle \simeq \frac{2q^2 Q_+^* p_{\alpha z}}{(eB_0)^2} \sum_{\beta} \sqrt{\mu_{\alpha\beta}} n_{\beta} \left[z \bar{z}_{\beta} \frac{\partial \ln(\bar{z}_{\beta} p_{\beta})}{\partial r} - \bar{z}_{\beta}^2 \frac{\partial \ln p_{\alpha z}}{\partial r} \right]$$

Note that in this approximation the electric field enters only via the electric drift velocity, which, since charge-independent, cancels out. Also $\sum_{\alpha, z} \langle z \Gamma_{\alpha z, r}^U \rangle = 0$ due to $\|\vec{B}$ momentum conservation in elastic collisions.

By summing over z we finally get the magnetic flux-surface averaged value of the total radial particle flux of the element α in the form

$$\langle \Gamma_{\alpha, r}^U \rangle \simeq \frac{2q^2 Q_+^* p_{\alpha}}{(eB_0)^2} \sum_{\beta} \sqrt{\mu_{\alpha\beta}} n_{\beta} \left[\bar{z}_{\alpha} \bar{z}_{\beta} \frac{\partial \ln(\bar{z}_{\beta} p_{\beta})}{\partial r} - \bar{z}_{\beta}^2 \frac{\partial \ln p_{\alpha}}{\partial r} \right]$$

We remark here that the equilibrium profiles of the total densities of the various ion species in a collision-dominated (PS) and source-free plasma region result from $\sum_z \langle \Gamma_{\alpha z, r} \rangle = 0$. Although this has to be performed in connection with the evaluation of the charge state distribution to yield the charge averaged values $\bar{z}_{\beta}, \bar{z}_{\beta}^2$ (note that $\bar{z}_{\beta}^2 \neq \bar{z}_{\beta}^2$), there are still numerical benefits of this method by a considerable reduction of the number of equations to be considered simultaneously.

III. Radial neoclassical fluxes resulting from $\|\vec{B}$ thermal forces

In order to include the effect of the thermal forces, we have to consider the additional effect of the heat fluxes in the collisional momentum transfer term $R_{\alpha z\parallel}$.

$$R_{\alpha z\parallel}^T = \sum_{\beta} \frac{\mu_{\alpha\beta}}{kT} I_{\alpha z} \bar{G}_{\alpha\beta}^{(2)} \left(\frac{h_{\alpha z\parallel}}{\rho_{\alpha z}} - \frac{\bar{h}_{\beta\parallel}}{\rho_{\beta}} \right) \quad ; \quad \rho_{\alpha z} = m_{\alpha} n_{\alpha z}$$

Whereas the longitudinal particle fluxes are coupled to the vertical particle drifts as described by the particle balance, the longitudinal heat fluxes are coupled to the vertical heat drifts as given by the energy balance (see ref. [4], p.21):

$$\begin{aligned} -\frac{\Theta}{rR} \frac{\partial(Rq_{\alpha z\parallel}^t)}{\partial\theta} &= -\nabla_v q_{\alpha z,v}^{nc} + \left(\frac{p_{\alpha z\perp}}{BR} - 2ze\Gamma_{\alpha z,v}^{nc} \right) \nabla_v \Phi + \frac{(\vec{\nabla} G_{\alpha z} \times \vec{\nabla} \Phi)_{\phi}}{B} - \\ &- ze\Gamma_{\alpha z\parallel} \nabla_{\parallel} \Phi + zeD_{\alpha z\perp} \frac{\partial n_{\alpha z}}{\partial r} \frac{\partial \Phi}{\partial r} + \frac{1}{rR} \frac{\partial}{\partial r} \left(rR D_{\alpha z\perp} \frac{\partial(G_{\alpha z} + p_{\alpha z\perp})}{\partial r} \right) + \delta Q_{\alpha z} \end{aligned}$$

The last two terms describe the divergence of the anomalous radial energy transport and the energy source due to inelastic collisions (the energy transfer between different ion species due to Coulomb collisions vanishes in the supposed case of temperature equilibration).

Moreover, we have used the following definitions: $G_{\alpha z} \equiv \frac{p_{\alpha z\parallel}^t}{2} + p_{\alpha z\perp}$

$$\begin{aligned} \begin{pmatrix} p_{\alpha z\parallel}^t \\ p_{\alpha z\perp} \end{pmatrix} &\equiv 2\pi \int_0^{+\infty} dv_{\perp} v_{\perp} \int_{-\infty}^{+\infty} dv_{\parallel} m_{\alpha} \begin{pmatrix} v_{\parallel}^2 \\ v_{\perp}^2/2 \end{pmatrix} F_{\alpha z}(\vec{x}, v_{\parallel}, v_{\perp}) \\ &\Rightarrow \begin{pmatrix} p_{\alpha z} \left(1 + \frac{2U_{\parallel}^2}{v_{T\alpha}^2} \right) \\ p_{\alpha z} \end{pmatrix} \end{aligned}$$

$$\begin{aligned}
\begin{pmatrix} q_{\alpha z||}^t \\ -q_{\alpha z,v}^{nc} \end{pmatrix} &\equiv 2\pi \int_0^{+\infty} dv_{\perp} v_{\perp} \int_{-\infty}^{+\infty} dv_{\parallel} \frac{m_{\alpha}}{2} (v_{\parallel}^2 + v_{\perp}^2) \begin{pmatrix} v_{\parallel} \\ \frac{v_{\parallel}^2 + v_{\perp}^2/2}{\Omega_{\alpha z} R} \end{pmatrix} F_{\alpha z}(\vec{x}, v_{\parallel}, v_{\perp}) \\
&\Rightarrow \begin{pmatrix} p_{\alpha z} \left(\frac{5}{2} + \frac{U_{\parallel}^2}{v_{T\alpha}^2} \right) U_{\parallel} \\ \frac{2p_{\alpha z} kT}{m_{\alpha} \Omega_{\alpha z} R} \left(\frac{5}{2} + \frac{9}{2} \frac{U_{\parallel}^2}{v_{T\alpha}^2} + \frac{U_{\parallel}^4}{v_{T\alpha}^4} \right) \end{pmatrix}
\end{aligned}$$

the arrows indicating the values calculated for a local shifted Maxwellian distribution function

$$F_{\alpha z}(\vec{x}, v_{\parallel}, v_{\perp}) = \frac{n_{\alpha z}}{(\sqrt{\pi} v_{T\alpha})^3} \exp \left[-\frac{(v_{\parallel} - U_{\parallel})^2 + v_{\perp}^2}{v_{T\alpha}^2} \right]$$

Since we are interested in the heat flux $h_{\alpha z||}$, we have, however, to take into account the deviation from the local shifted Maxwellian distribution function. Relating the thermal fluxes, as before, to a coordinate system moving with $U_{\parallel}$, we have

$$q_{\alpha z||}^t = h_{\alpha z||} + \left(\frac{5}{2} kT + \frac{3}{2} m_{\alpha} U_{\parallel}^2 \right) n_{\alpha z} w_{\alpha z||} + p_{\alpha z} \left(\frac{5}{2} + \frac{U_{\parallel}^2}{v_{T\alpha}^2} \right) U_{\parallel}$$

Note that the last term disappears in the difference $h_{\alpha z||}/\rho_{\alpha z} - h_{\beta z||}/\rho_{\beta z}$. Going again to the limit $U_{\parallel}^2/v_{T\alpha}^2 \ll 1$ and neglecting anomalous transport and source terms, we obtain the approximation

$$\begin{aligned}
-\frac{\Theta}{rR} \frac{\partial(Rh_{\alpha z||})}{\partial\theta} &\simeq -\frac{\Theta}{rR} \frac{\partial}{\partial\theta} \left(Rq_{\alpha z||}^t - \frac{5}{2} kT R\Gamma_{\alpha z||} \right) \simeq \frac{5p_{\alpha z}}{m_{\alpha} \Omega_{\alpha z} R} \nabla_v(kT) + \\
&+ \left[\left(\frac{5}{2} n_{\alpha z} \vec{\nabla}(kT) - \vec{\nabla}p_{\alpha z} \right) \times \frac{\vec{\nabla}\Phi}{B} \right]_{\phi} - \nabla_{\parallel} \left(ze\Phi + \frac{5}{2} kT \right) \Gamma_{\alpha z||}
\end{aligned}$$

Considering the first term on the rhs of this equation to be the dominant one, we perform again the θ -integration with the result that for $r/R_0 \ll 1$

$$h_{\alpha z||} \simeq \frac{5p_{\alpha z} r \cos \theta}{m_{\alpha} \Omega_{\alpha z} \Theta R} \frac{\partial(kT)}{\partial r}$$

Inserting this expression into the heat flux contribution to $R_{\alpha z||}$ and its connection with the radial neoclassical particle flux, we get (with $g^{(2)}(m_{\alpha}/m_{\beta}) = 3/5 \rightarrow$ see p.3)

$$\Gamma_{\alpha z, r}^T \simeq \frac{3r \cos \theta}{(eB\Theta)^2 R} Q_+^* p_{\alpha z} \sum_{\beta} \sqrt{\mu_{\alpha\beta}}^3 n_{\beta} \left(\frac{\bar{z}_{\beta}^2}{m_{\alpha}} - \frac{z \bar{z}_{\beta}}{m_{\beta}} \right) \frac{\partial \ln T}{\partial r}$$

$$\text{and } \langle \Gamma_{\alpha z, r}^T \rangle \simeq \frac{3q^2 Q_+^* p_{\alpha z}}{(eB_0)^2} \sum_{\beta} \sqrt{\mu_{\alpha\beta}}^3 n_{\beta} \left(\frac{\bar{z}_{\beta}^2}{m_{\alpha}} - \frac{z \bar{z}_{\beta}}{m_{\beta}} \right) \frac{\partial \ln T}{\partial r}$$

$$\langle \Gamma_{\alpha, r}^T \rangle \simeq \frac{3q^2 Q_+^* p_{\alpha}}{(eB_0)^2} \sum_{\beta} \sqrt{\mu_{\alpha\beta}}^3 n_{\beta} \left(\frac{\bar{z}_{\beta}^2}{m_{\alpha}} - \frac{\bar{z}_{\alpha} \bar{z}_{\beta}}{m_{\beta}} \right) \frac{\partial \ln T}{\partial r}$$

$$\text{Again } \sum_{\alpha, z} \langle z \Gamma_{\alpha z, r}^T \rangle \sim \sum_{\alpha, \beta} \sqrt{\mu_{\alpha\beta}}^3 n_{\alpha} n_{\beta} \left(\frac{\bar{z}_{\alpha} \bar{z}_{\beta}^2}{m_{\alpha}} - \frac{\bar{z}_{\alpha}^2 \bar{z}_{\beta}}{m_{\beta}} \right) = 0 \quad \text{holds.}$$

IV. Radial neoclassical fluxes in the 13-moment approximation

Adding the contributions from friction (upper index U) and thermal (upper index T) forces, we finally arrive at the formula (in the 13-moment approximation)

$$\begin{aligned} \langle \Gamma_{\alpha z, r} \rangle = \langle \frac{R_{\alpha z||}}{m_{\alpha} \Theta \Omega_{\alpha z}} \rangle \simeq & - \frac{2q^2 Q_+^* p_{\alpha z}}{(eB_0)^2} \sum_{\beta} \sqrt{\mu_{\alpha\beta}} n_{\beta} \bar{z}_{\beta}^2 \left[\left(\frac{\partial \ln p_{\alpha z}}{\partial r} - \right. \right. \\ & \left. \left. - \frac{z \bar{z}_{\beta}}{\bar{z}_{\beta}^2} \frac{\partial \ln(\bar{z}_{\beta} p_{\beta})}{\partial r} \right) - \frac{3}{2} \frac{\mu_{\alpha\beta}}{m_{\alpha}} \left(1 - \frac{m_{\alpha}}{m_{\beta}} \frac{z \bar{z}_{\beta}}{\bar{z}_{\beta}^2} \right) \frac{\partial \ln T}{\partial r} \right] \end{aligned}$$

$$\begin{aligned}
\langle \Gamma_{\alpha,r} \rangle \simeq & - \frac{2q^2 Q_+^* p_\alpha}{(eB_0)^2} \sum_{\beta} \sqrt{\mu_{\alpha\beta}} n_{\beta} z_{\beta}^{-2} \left[\left(\frac{\partial \ln p_{\alpha}}{\partial r} - \frac{\bar{z}_{\alpha} \bar{z}_{\beta}}{z_{\beta}^2} \frac{\partial \ln(\bar{z}_{\beta} p_{\beta})}{\partial r} \right) - \right. \\
& \left. - \frac{3}{2} \frac{\mu_{\alpha\beta}}{m_{\alpha}} \left(1 - \frac{m_{\alpha}}{m_{\beta}} \frac{\bar{z}_{\alpha} \bar{z}_{\beta}}{z_{\beta}^2} \right) \frac{\partial \ln T}{\partial r} \right]
\end{aligned}$$

The last expression is exactly the same as in ref.[6], but differs from the one given by equ.(26) of ref.[7] (identifying, in our notation, α with the trace impurity component I and β with the main impurity species A) even if one goes to the limit $m_{\alpha}/m_{\beta} \rightarrow \infty$ setting in ref.[7] $c_0 = 1$, $c_1 = 5\sqrt{2}/8$, $c_2 = 0$ and neglects 2.86 compared to $5.79 z_{\beta}^2 z_{\beta}^{-2}$. The important discrepancy is that in the thermal force contribution of ref.[7] instead of $\bar{z}_{\beta}$ the expression $z_{\beta}^{-1}/z_{\beta}^{-2}$ appears. Neither in ref.[6] nor within the framework of the present theory terms $\sim z_{\beta}^{-k}$ appear in the radial fluxes, not even in higher order approximations (see below). Comparison with the expressions of ref.[8] describing as those in [6] the Coulomb interaction between trace amounts of Mo ions with C as the main impurity species shows that the charge state number of carbon is to be understood as an effective charge, which usually is space-dependent. The corresponding derivative with respect to the radius is, however, missing. Therefore both references [7] and [8] present incorrect expressions for $\langle \Gamma_{\alpha r} \rangle$.

Considering only interactions between the different charge states of a single impurity element (i.e. for the index $\alpha = \beta$, which is therefore omitted from the following formula) and separating the contributions of the density gradients from those $\sim \partial \ln T / \partial r$, we obtain

$$\begin{aligned}
\langle \Gamma_{z,r} \rangle \simeq & - \frac{2q^2 Q_+^* p_z}{(eB_0)^2} \sqrt{\frac{m_z}{2}} \left[\sum_{z' \neq z} \left(z' \frac{\partial \ln n_z}{\partial r} - z \frac{\partial \ln n_{z'}}{\partial r} \right) z' n_{z'} + \right. \\
& \left. + \sum_{z' \neq z} z'(z - z') n_{z'} \left(\frac{3}{4} - 1 \right) \frac{\partial \ln T}{\partial r} \right]
\end{aligned}$$

the first contribution in the underlined bracket resulting from the thermal force (p.10), the second one from the friction force (p.7). The total

expression exactly equals the one given in ref.[5], equ.(4), noticing that $\nu_{zp}^c \equiv z^2 n_p \sqrt{m_p} Q_+^* / m_z$. Apart from the factor $2q^2$ it is exactly the formula, which one derives from the classical transport theory in the 13-moment approximation of the ion distribution functions.

In a similar way we get, within the 13-moment approximation, the following expressions for the $\|\vec{B}$ collisional heat transport and the attributed magnetic flux surface averaged heat fluxes:

$$\begin{aligned}
\langle h_{\alpha z, r} \rangle &= \langle \frac{H_{\alpha z \|}}{\Theta \Omega_{\alpha z}} \rangle \simeq \frac{3q^2 Q_+^* p_{\alpha z} kT}{(eB_0)^2} \sum_{\beta} \frac{\sqrt{\mu_{\alpha\beta}}^3}{m_{\alpha}} n_{\beta} \bar{z}_{\beta}^2 \left[\left(\frac{\partial \ln p_{\alpha z}}{\partial r} - \right. \right. \\
&\quad \left. \left. - \frac{z \bar{z}_{\beta}}{\bar{z}_{\beta}^2} \frac{\partial \ln(\bar{z}_{\beta} p_{\beta})}{\partial r} \right) - \frac{9}{2} \frac{\mu_{\alpha\beta}}{m_{\beta}} \left(\frac{g_{\alpha\beta}^{(4)}}{g_{\alpha\beta}^{(5)}} - \frac{z \bar{z}_{\beta}}{\bar{z}_{\beta}^2} \right) \frac{\partial \ln T}{\partial r} \right] \\
\langle h_{\alpha, r} \rangle &\simeq \frac{3q^2 Q_+^* p_{\alpha} kT}{(eB_0)^2} \sum_{\beta} \frac{\sqrt{\mu_{\alpha\beta}}^3}{m_{\alpha}} n_{\beta} \bar{z}_{\beta}^2 \left[\left(\frac{\partial \ln p_{\alpha}}{\partial r} - \frac{\bar{z}_{\alpha} \bar{z}_{\beta}}{\bar{z}_{\beta}^2} \frac{\partial \ln(\bar{z}_{\beta} p_{\beta})}{\partial r} \right) - \right. \\
&\quad \left. - \frac{9}{2} \frac{\mu_{\alpha\beta}}{m_{\beta}} \left(\frac{g_{\alpha\beta}^{(4)}}{g_{\alpha\beta}^{(5)}} - \frac{\bar{z}_{\alpha} \bar{z}_{\beta}}{\bar{z}_{\beta}^2} \right) \frac{\partial \ln T}{\partial r} \right]
\end{aligned}$$

where we have used the relations for $\bar{G}_{\alpha\beta}^{(n)}$ and $g_{\alpha\beta}^{(n)}$ as given in the Appendix. In particular $g_{\alpha\beta}^{(5)}/g_{\alpha\beta}^{(2)} = -9\mu_{\alpha\beta}^2/(2m_{\alpha}m_{\beta})$

As in the case of the radial particle flux the total radial heat flux $\langle h_{\alpha, r} \rangle$ follows from the individual radial heat fluxes $\langle h_{\alpha z, r} \rangle$ by replacing z , $n_{\alpha z}$ and $p_{\alpha z}$ with $\bar{z}_{\alpha}$, n_{α} and p_{α} respectively. It should be mentioned that again these expressions exactly agree with those given in ref.[6].

V. Radial neoclassical fluxes in the 21-moment approximation

In order to proceed to the 21-moment approximation of the ion distribution functions, we have still to include the contribution

$$R_{\alpha z||}^S = \sum_{\beta} \left(\frac{\mu_{\alpha\beta}}{kT} \right)^2 I_{\alpha z} \bar{G}_{\alpha\beta}^{(3)} \left(\frac{r_{\alpha z||}}{\rho_{\alpha z}} - \frac{\bar{r}_{\beta||}}{\rho_{\beta}} \right)$$

and transform it according to the procedure given on p.4 such that

$$R_{\alpha z||}^S = \sum_{\beta} \left(\frac{\mu_{\alpha\beta}}{kT} \right)^2 I_{\alpha z} \bar{G}_{\alpha\beta}^{(3)} \left(\frac{\bar{r}_{\alpha||}}{\rho_{\alpha}} - \frac{\bar{r}_{\beta||}}{\rho_{\beta}} - \frac{(kT)^2}{m_{\alpha}^2 S_{\alpha}^{(8)}} \left[S_{\alpha}^{(3)} \left(\frac{\Gamma_{\alpha z||}}{n_{\alpha z}} - \frac{\bar{\Gamma}_{\alpha||}}{n_{\alpha}} \right) + 7 S_{\alpha}^{(6)} \left(\frac{h_{\alpha z||}}{p_{\alpha z}} - \frac{\bar{h}_{\alpha||}}{p_{\alpha}} \right) \right] \right)$$

The moments $\bar{r}_{\alpha||}$ can be evaluated in terms of the charge-averaged particle and heat fluxes $\bar{\Gamma}_{\alpha||}$ respectively $\bar{h}_{\alpha||}$ by the following reduced set of equations

$$\sum_{\beta} \left[c_{\alpha\beta}^{(31)} m_{\beta} \bar{\Gamma}_{\beta||} + c_{\alpha\beta}^{(32)} \bar{h}_{\beta||} + c_{\alpha\beta}^{(33)} \bar{r}_{\beta||} \right] = 0$$

which, by Cramer's rule, has the formal solution (see p.3)

$$\bar{r}_{\delta||} = \frac{| c_{\gamma\kappa}^{(33)} (1 - \delta_{\kappa\delta}) - \sum_{\epsilon} [c_{\gamma\epsilon}^{(31)} m_{\epsilon} \bar{\Gamma}_{\epsilon||} + c_{\gamma\epsilon}^{(32)} \bar{h}_{\epsilon||}] \delta_{\kappa\delta} |}{| c_{\gamma\kappa}^{(33)} |}$$

In these equations the identities $\Gamma_{\alpha z||} \equiv n_{\alpha z}(w_{\alpha z||} + U_{||})$ and $\bar{\Gamma}_{\alpha||} \equiv n_{\alpha}(\bar{w}_{\alpha||} + U_{||})$ have been used for the substitutions

$$w_{\alpha z||} - \bar{w}_{\alpha||} = \frac{\Gamma_{\alpha z||}}{n_{\alpha z}} - \frac{\bar{\Gamma}_{\alpha||}}{n_{\alpha}} \quad \text{and} \quad \sum_{\beta} c_{\alpha\beta}^{(31)} \rho_{\beta} \bar{w}_{\beta||} = \sum_{\beta} c_{\alpha\beta}^{(31)} m_{\beta} \bar{\Gamma}_{\beta||}$$

where the second equality follows from the relation

$$\sum_{\beta} c_{\alpha\beta}^{(31)} \rho_{\beta} = \sum_{\beta} \frac{\mu_{\alpha\beta}^2 \bar{G}_{\alpha\beta}^{(3)} - \delta_{\alpha\beta} \sum_{\kappa} \mu_{\alpha\kappa}^2 \bar{G}_{\alpha\kappa}^{(3)}}{\rho_{\alpha} (kT)^2} = 0$$

The formulation of the 21-moment approximation of the neoclassical particle flux, averaged over a magnetic flux surface, can now be closed by substituting in the above equations the longitudinal particle and heat fluxes $\Gamma_{\alpha z||}$ and $h_{\alpha z||}$ respectively by the radial pressure and temperature gradients, with the result that

$$\langle \Gamma_{\alpha z, r}^S \rangle \simeq -\frac{3q^2 Q^* p_{\alpha z}}{7(eB_0)^2} \sum_{\beta} \sqrt{\mu_{\alpha\beta}} n_{\beta} \bar{z}_{\beta}^2 \left[\left(\frac{\mu_{\alpha\beta}}{kT} \right)^2 \frac{z[I]}{kT} - \left(\frac{\mu_{\alpha\beta}}{m_{\alpha}} \right)^2 [II] \right]$$

$$[I] = \frac{|c_{\gamma\kappa}^{(33)}(1 - \delta_{\kappa\alpha}) - f_{\gamma}\delta_{\kappa\alpha}|}{\rho_{\alpha}|c_{\gamma\kappa}^{(33)}|} - \frac{|c_{\gamma\kappa}^{(33)}(1 - \delta_{\kappa\beta}) - f_{\gamma}\delta_{\kappa\beta}|}{\rho_{\beta}|c_{\gamma\kappa}^{(33)}|}$$

$$\text{with } f_{\gamma} \equiv \sum_{\epsilon} \frac{\bar{z}_{\epsilon} p_{\epsilon}}{z_{\epsilon}^2} \left[m_{\epsilon} c_{\gamma\epsilon}^{(31)} \frac{\partial \ln(\bar{z}_{\epsilon} p_{\epsilon})}{\partial r} + \frac{5}{2} kT c_{\gamma\epsilon}^{(32)} \frac{\partial \ln T}{\partial r} \right]$$

$$[II] = \frac{35}{2} \left[\frac{\sum_{\kappa} \mu_{\alpha\kappa}^2 \bar{G}_{\alpha\kappa}^{(3)}}{m_{\alpha}^2 \sum_{\kappa} \bar{G}_{\alpha\kappa}^{(8)}} \left(\frac{\partial \ln p_{\alpha z}}{\partial r} - \frac{z \bar{z}_{\alpha}}{z_{\alpha}^2} \frac{\partial \ln(\bar{z}_{\alpha} p_{\alpha})}{\partial r} \right) + \right. \\ \left. + \frac{\sum_{\kappa} \mu_{\alpha\kappa} \bar{G}_{\alpha\kappa}^{(6)}}{m_{\alpha} \sum_{\kappa} \bar{G}_{\alpha\kappa}^{(8)}} \left(1 - \frac{z \bar{z}_{\alpha}}{z_{\alpha}^2} \right) \frac{\partial \ln T}{\partial r} \right]$$

where the radial electric field again drops out due to the above mentioned relation $\sum_{\beta} c_{\alpha\beta}^{(31)} \rho_{\beta} = 0$. We used the relation $g_{\alpha\beta}^{(3)} = (3/14)g_{\alpha\beta}^{(1)}$ (see Appendix) and substituted the coefficients $S_{\alpha}^{(k)}$ from ref.[1].

Summarizing the various contributions (upper indices U, T, S) to the magnetic surface averaged radial particle flux of the ion species α in charge state z , we finally obtain the expression (in the 21-moment approximation)

$$\langle \Gamma_{\alpha z, r} \rangle \simeq -\frac{2q^2 Q^* p_{\alpha z}}{(eB_0)^2} \sum_{\beta} \sqrt{\mu_{\alpha\beta}} n_{\beta} \bar{z}_{\beta}^2 \left[\left(\frac{\partial \ln p_{\alpha z}}{\partial r} - \frac{z \bar{z}_{\beta}}{z_{\beta}^2} \frac{\partial \ln(\bar{z}_{\beta} p_{\beta})}{\partial r} \right) - \right.$$

$$\begin{aligned}
& -\frac{3}{2} \frac{\mu_{\alpha\beta}}{m_\alpha} \left(1 - \frac{m_\alpha}{m_\beta} \frac{z\bar{z}_\beta}{\bar{z}_\beta^2}\right) \frac{\partial \ln T}{\partial r} - \frac{15}{4} \frac{\mu_{\alpha\beta}^2 \sum_\kappa \mu_{\alpha\kappa}^2 \bar{G}_{\alpha\kappa}^{(3)}}{m_\alpha^4 \sum_\kappa \bar{G}_{\alpha\kappa}^{(8)}} \left(\frac{\partial \ln p_{\alpha z}}{\partial r} \right. \\
& \left. - \frac{z\bar{z}_\alpha}{\bar{z}_\alpha^2} \frac{\partial \ln(\bar{z}_\alpha p_\alpha)}{\partial r} \right) - \frac{15}{4} \frac{\mu_{\alpha\beta}^2 \sum_\kappa \mu_{\alpha\kappa} \bar{G}_{\alpha\kappa}^{(6)}}{m_\alpha^3 \sum_\kappa \bar{G}_{\alpha\kappa}^{(8)}} \left(1 - \frac{z\bar{z}_\alpha}{\bar{z}_\alpha^2}\right) \frac{\partial \ln T}{\partial r} + \frac{3}{14} \left(\frac{\mu_{\alpha\beta}}{kT}\right)^2 \frac{z[I]}{kT} \Big]
\end{aligned}$$

Inserting the values for $\bar{G}_{\alpha\beta}^{(n)}$ (see Appendix) we get

$$\frac{15}{4} \frac{\mu_{\alpha\beta}^2 \sum_\kappa \mu_{\alpha\kappa}^2 \bar{G}_{\alpha\kappa}^{(3)}}{m_\alpha^4 \sum_\kappa \bar{G}_{\alpha\kappa}^{(8)}} = \frac{3}{35} \frac{\mu_{\alpha\beta}^2 \sum_\kappa \sqrt{\mu_{\alpha\kappa}}^5 \bar{z}_\kappa^2 n_\kappa}{m_\alpha^4 \sum_\kappa \frac{g_{\alpha\kappa}^{(8)}}{g_{\alpha\kappa}^{(9)}} \frac{\sqrt{\mu_{\alpha\kappa}}^5}{(m_\alpha + m_\kappa)^2} \bar{z}_\kappa^2 n_\kappa}$$

$$\text{and} \quad \frac{15}{4} \frac{\mu_{\alpha\beta}^2 \sum_\kappa \mu_{\alpha\kappa} \bar{G}_{\alpha\kappa}^{(6)}}{m_\alpha^3 \sum_\kappa \bar{G}_{\alpha\kappa}^{(8)}} = -\frac{9}{14} \frac{\mu_{\alpha\beta}^2 \sum_\kappa \frac{g_{\alpha\kappa}^{(6)}}{g_{\alpha\kappa}^{(7)}} \frac{\sqrt{\mu_{\alpha\kappa}}^5}{m_\alpha + m_\kappa} \bar{z}_\kappa^2 n_\kappa}{m_\alpha^3 \sum_\kappa \frac{g_{\alpha\kappa}^{(8)}}{g_{\alpha\kappa}^{(9)}} \frac{\sqrt{\mu_{\alpha\kappa}}^5}{(m_\alpha + m_\kappa)^2} \bar{z}_\kappa^2 n_\kappa}$$

Again, $\langle \Gamma_{\alpha z, r} \rangle$ passes into $\langle \Gamma_{\alpha, r} \rangle$ by the substitutions $p_{\alpha z} \rightarrow p_\alpha$ and $z \rightarrow \bar{z}_\alpha$.

Similarly, in the 21-moment approximation, the additional term

$$\begin{aligned}
H_{\alpha z||}^S &= \sum_\beta \frac{\mu_{\alpha\beta}}{m_\alpha} I_{\alpha z} \bar{G}_{\alpha\beta}^{(6)} \left(\frac{r_{\alpha z||}}{p_{\alpha z}} - \frac{g_{\alpha\beta}^{(7)}}{g_{\alpha\beta}^{(6)}} \frac{\bar{r}_{\beta||}}{p_\beta} \right) = \\
& \sum_\beta \frac{\mu_{\alpha\beta}}{kT} I_{\alpha z} \bar{G}_{\alpha\beta}^{(6)} \left(\frac{\bar{r}_{\alpha||}}{\rho_\alpha} - \frac{m_\beta g_{\alpha\beta}^{(7)}}{m_\alpha g_{\alpha\beta}^{(6)}} \frac{\bar{r}_{\beta||}}{\rho_\beta} \right)
\end{aligned}$$

$$-\frac{(kT)^2}{m_\alpha^2 S_\alpha^{(8)}} \left[S_\alpha^{(3)} \left(\frac{\Gamma_{\alpha z}}{n_{\alpha z}} - \frac{\bar{\Gamma}_{\alpha}}{n_\alpha} \right) + 7 S_\alpha^{(6)} \left(\frac{h_{\alpha z}}{p_{\alpha z}} - \frac{\bar{h}_\alpha}{p_\alpha} \right) \right]$$

arises in the $\|\vec{B}$ collisional heat transport. Following the procedure mentioned on p.14 we get the additional contribution to the individual radial heat flux

$$< h_{\alpha z, r}^S > \simeq$$

$$-\frac{3q^2 Q_+^* p_{\alpha z} kT}{7(eB_0)^2} \sum_\beta \frac{m_\alpha g_{\alpha\beta}^{(6)}}{\mu_{\alpha\beta} g_{\alpha\beta}^{(3)}} \sqrt{\mu_{\alpha\beta}} n_\beta \bar{z}_\beta^2 \left[\left(\frac{\mu_{\alpha\beta}}{kT} \right)^2 \frac{z[I]^*}{kT} - \left(\frac{\mu_{\alpha\beta}}{m_\alpha} \right)^2 [II] \right]$$

$$\text{where } [I]^* = \frac{|c_{\gamma\kappa}^{(33)}(1 - \delta_{\kappa\alpha}) - f_\gamma \delta_{\kappa\alpha}|}{\rho_\alpha |c_{\gamma\kappa}^{(33)}|} - \frac{m_\beta g_{\alpha\beta}^{(7)}}{m_\alpha g_{\alpha\beta}^{(6)}} \frac{|c_{\gamma\kappa}^{(33)}(1 - \delta_{\kappa\beta}) - f_\gamma \delta_{\kappa\beta}|}{\rho_\beta |c_{\gamma\kappa}^{(33)}|}$$

Adding the various contributions (upper indices U, T, S) to the magnetic surface averaged radial heat flux of the ion species α in charge state z , we finally get the expression (in the 21-moment approximation)

$$\begin{aligned} < h_{\alpha z, r} > \simeq \frac{2q^2 Q_+^* p_{\alpha z} kT}{(eB_0)^2} \sum_\beta \frac{\sqrt{\mu_{\alpha\beta}}^3}{m_\alpha} n_\beta \bar{z}_\beta^2 \left[\frac{3}{2} \left(\frac{\partial \ln p_{\alpha z}}{\partial r} - \frac{z \bar{z}_\beta}{\bar{z}_\beta^2} \frac{\partial \ln(\bar{z}_\beta p_\beta)}{\partial r} \right) - \right. \\ & - \frac{27}{4} \frac{\mu_{\alpha\beta}}{m_\beta} \left(\frac{g_{\alpha\beta}^{(4)}}{g_{\alpha\beta}^{(5)}} - \frac{z \bar{z}_\beta}{\bar{z}_\beta^2} \right) \frac{\partial \ln T}{\partial r} + \frac{15}{4} \frac{g_{\alpha\beta}^{(6)}}{g_{\alpha\beta}^{(3)} m_\alpha^2} \sum_\kappa \mu_{\alpha\kappa}^2 \bar{G}_{\alpha\kappa}^{(3)} \left(\frac{\partial \ln p_{\alpha z}}{\partial r} - \frac{z \bar{z}_\alpha}{\bar{z}_\alpha^2} \frac{\partial \ln(\bar{z}_\alpha p_\alpha)}{\partial r} \right) + \\ & \left. + \frac{15}{4} \frac{g_{\alpha\beta}^{(6)}}{g_{\alpha\beta}^{(3)} m_\alpha} \sum_\kappa \mu_{\alpha\kappa} \bar{G}_{\alpha\kappa}^{(6)} \left(1 - \frac{z \bar{z}_\alpha}{\bar{z}_\alpha^2} \right) \frac{\partial \ln T}{\partial r} - \frac{3}{14} \frac{g_{\alpha\beta}^{(6)}}{g_{\alpha\beta}^{(3)}} \left(\frac{m_\alpha}{kT} \right)^2 \frac{z[I]^*}{kT} \right] \end{aligned}$$

recalling the relations on p.14/15 and
$$\frac{g_{\alpha\beta}^{(6)}}{g_{\alpha\beta}^{(3)}} = -\frac{15}{2} \frac{\mu_{\alpha\beta}^2 g_{\alpha\beta}^{(6)}}{m_{\alpha} m_{\beta} g_{\alpha\beta}^{(7)}} < 0$$

Again, $\langle h_{\alpha z, r} \rangle$ passes into $\langle h_{\alpha, r} \rangle$ by the substitutions $p_{\alpha z} \rightarrow p_{\alpha}$ and $z \rightarrow \bar{z}_{\alpha}$. Note that $\langle \Gamma_{\alpha z, r} \rangle$ and $\langle h_{\alpha z, r} \rangle$ have opposite signs in the transport coefficients (both in the temperature gradient and in the pressure gradient terms), which reflects the corresponding effects in the classical collisional $\|\vec{B}$ transport (the effects of both velocity differences and temperature gradients have different signs in particle and heat flows, see for instance ref.[9]). Since the radial particle and heat fluxes are influenced by the various processes with different weights, they are not necessarily counterdirected. Moreover, the total heat flux for $U_{\parallel} = 0$ is $\langle q_{\alpha z, r} \rangle = \langle h_{\alpha z, r} \rangle + (5/2)kT \langle \Gamma_{\alpha z, r} \rangle$ and is therefore correlated with the particle flux.

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Acknowledgement

One of the authors (B.F.Mohamed) would like to thank the members of the IPP/KFA Jülich for their hospitality during his visit and the INT Büro for the financial support.

Appendix

By definition we have

$$\bar{G}_{\alpha\beta}^{(n)} \equiv \sum_{z,\zeta} G_{\alpha z, \beta \zeta}^{(n)} = Q_+^* g_{\alpha\beta}^{(n)} \sqrt{\mu_{\alpha\beta}} n_\alpha n_\beta \bar{z}_\alpha^2 \bar{z}_\beta^2$$

$$\text{where } Q_+^* = \frac{4\sqrt{2}\pi}{3} \left(\frac{e^2}{4\pi\epsilon_0} \right)^2 \frac{\ln \Lambda}{\sqrt{kT}^3} \quad \text{and} \quad g_{\alpha\beta}^{(n)} = g^{(n)} \left(\frac{m_\alpha}{m_\beta} \right)$$

By comparison with the expressions given in ref.[1] we have

$$g_{\alpha\beta}^{(1)} = -1 \quad ; \quad g_{\alpha\beta}^{(2)} = \frac{3}{5} \quad ; \quad g_{\alpha\beta}^{(3)} = -\frac{3}{14}$$

$$g_{\alpha\beta}^{(4)} = -\left(\frac{13}{10} \frac{m_\beta}{m_\alpha} + \frac{8}{5} + 3 \frac{m_\alpha}{m_\beta} \right) \frac{\mu_{\alpha\beta}^2}{m_\alpha m_\beta} \quad ; \quad g_{\alpha\beta}^{(5)} = -\frac{27}{10} \frac{\mu_{\alpha\beta}^2}{m_\alpha m_\beta}$$

$$g_{\alpha\beta}^{(6)} = \frac{3}{5} \left(\frac{23}{28} \frac{m_\beta}{m_\alpha} + \frac{8}{7} + 3 \frac{m_\alpha}{m_\beta} \right) \frac{\mu_{\alpha\beta}^2}{m_\alpha m_\beta} \quad ; \quad g_{\alpha\beta}^{(7)} = \frac{45}{28} \frac{\mu_{\alpha\beta}^2}{m_\alpha m_\beta}$$

$$g_{\alpha\beta}^{(8)} = -\left(\frac{433}{280} \frac{m_\beta^2}{m_\alpha^2} + \frac{139}{35} \frac{m_\beta}{m_\alpha} + \frac{459}{35} + \frac{32}{5} \frac{m_\alpha}{m_\beta} + 5 \frac{m_\alpha^2}{m_\beta^2} \right) \frac{\mu_{\alpha\beta}^4}{(m_\alpha m_\beta)^2}$$

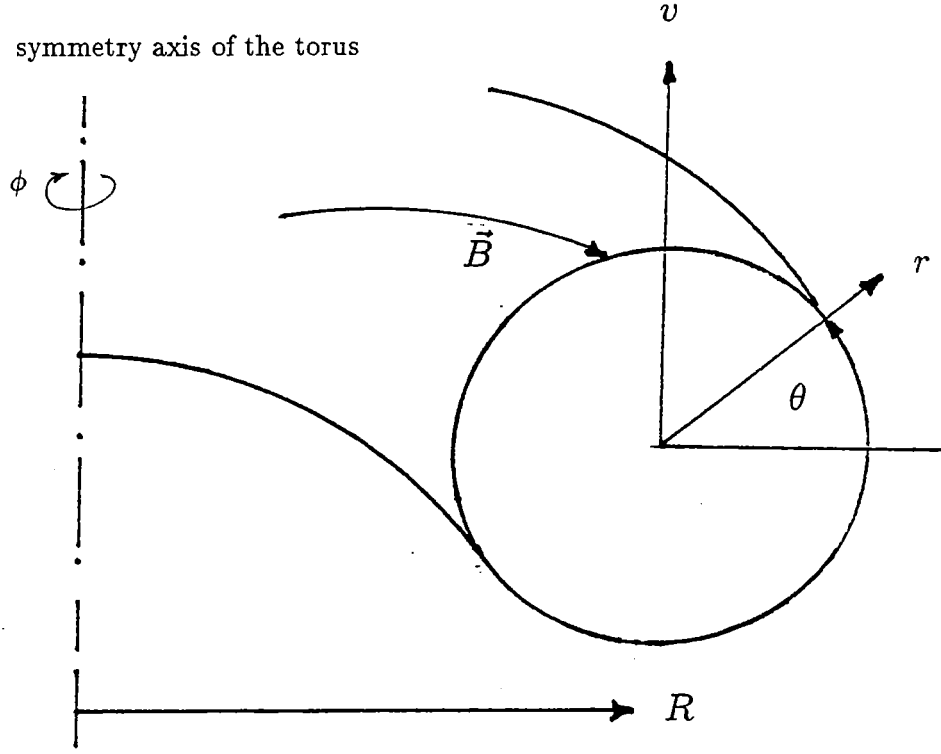
$$g_{\alpha\beta}^{(9)} = -\frac{75}{8} \frac{\mu_{\alpha\beta}^4}{(m_\alpha m_\beta)^2}$$

We recall from ref.[1] that

$$S_\alpha^{(2)} = \frac{5}{2} \sum_\kappa \frac{\mu_{\alpha\kappa}}{m_\alpha} \bar{G}_{\alpha\kappa}^{(2)} \quad ; \quad S_\alpha^{(3)} = \frac{35}{2} \sum_\kappa \left(\frac{\mu_{\alpha\kappa}}{m_\alpha} \right)^2 \bar{G}_{\alpha\kappa}^{(3)}$$

$$S_\alpha^{(6)} = \sum_\kappa \frac{\mu_{\alpha\kappa}}{m_\alpha} \bar{G}_{\alpha\kappa}^{(6)} \quad ; \quad S_\alpha^{(k)} = \sum_\kappa \bar{G}_{\alpha\kappa}^{(k)} \quad \text{for } k = 1, 4, 8$$

fig.1: Coordinate system and standard magnetic field



$$\nabla_v \equiv \cos \theta \frac{\partial}{r \partial \theta} + \sin \theta \frac{\partial}{\partial r}$$

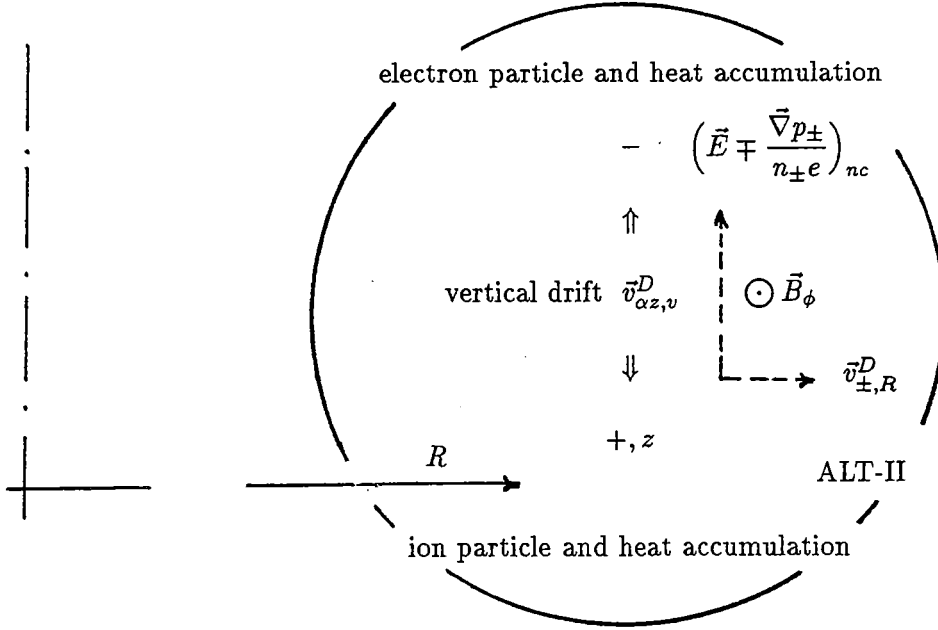
$$\vec{B} = (0, -\Theta, 1) B_\phi$$

$$\text{with } B_\phi R = \text{const. and } \Theta = -\frac{B_\theta}{B_\phi} = \Theta(r) > 0$$

fig.2: Physics of the nc-transport

(a) driving mechanism of vertical centrifugal and $\vec{\nabla} B$ drift

$$\vec{v}_{\alpha z, v}^D = - \frac{(p_{\parallel} + p_{\perp})_{\alpha z} \vec{\nabla} \ln B \times \vec{B}}{n_{\alpha z} z e B^2} \text{ assuming } \text{rot} \vec{B} = 0$$



nc-transport: horizontal particle and heat drifts due to the vertical potential, density and temperature gradients

$$n_{\alpha z} \vec{v}_{\alpha z \perp}^D = \frac{(n_{\alpha z} z e \vec{E} - \vec{\nabla} p_{\alpha z}) \times \vec{B}}{z e B^2} \text{ and } \vec{h}_{\alpha z \perp}^D = - \frac{5}{2} p_{\alpha z} \frac{\vec{\nabla}(kT) \times \vec{B}}{z e B^2}$$

$$\text{for 1D-model: } \langle n_{\alpha z} v_{\alpha z, r}^D, h_{\alpha z, r}^D \rangle = \frac{\oint (n_{\alpha z} v_{\alpha z, r}^D, h_{\alpha z, r}^D) df}{\oint df}$$

where $\langle .. \rangle$ denotes averaging over a magnetic flux surface.

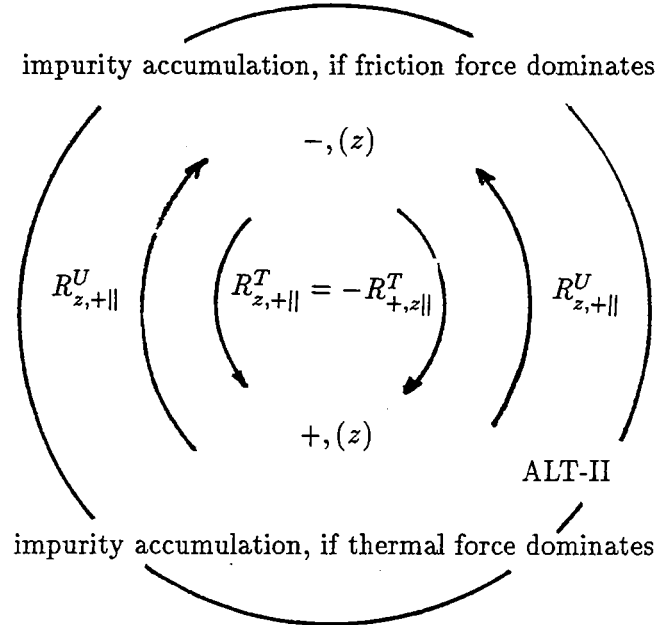
fig.2: Physics of the nc-transport

(b) dynamic equilibrium via $\|\vec{B}$ momentum and heat flux balance

$$n_{\alpha z} z e E_{\parallel} - \nabla_{\parallel} p_{\alpha z} + R_{\alpha z \parallel} \simeq 0 \quad ; \quad -\frac{5p_{\alpha z}}{2m_{\alpha}} \nabla_{\parallel} (kT) + H_{\alpha z \parallel} \simeq 0$$

subject to the particle and energy balance in an axisymmetric plasma

$R_{\alpha z \parallel} = R_{\alpha z \parallel}^U + R_{\alpha z \parallel}^T$ is the sum of friction and thermal forces



shown for a single combination of charge state and impurity element,

i.e. for $\alpha z \rightarrow z$ with $R_{z,+||} = -R_{+,z||}$.

Note that the vertical pressure gradient of z reverses sign, if the corresponding thermal force becomes larger than the friction force (temperature screening of the plasma core from that impurity species in the trace impurity limit).

fig.3: Basic relations for neoclassical transport.

1. toroidal components of momentum and heat flux equations for axisymmetric systems $\Rightarrow$ radial flux- $\|\vec{B}$ friction relations

$$\Gamma_{\alpha z, r} = \frac{R_{\alpha z \parallel}}{m_{\alpha} \Theta \Omega_{\alpha z}} \quad \text{and} \quad h_{\alpha z, r} = \frac{H_{\alpha z \parallel}}{\Theta \Omega_{\alpha z}}$$

with the magnetic surface averages $\langle \dots \rangle \equiv \oint \frac{d\theta}{2\pi} \frac{R}{R_0} \dots$

2. $\|\vec{B}$ flux-friction relations (in the 13 moment approximation [1])

$$R_{\alpha z \parallel} \simeq \sum_{\beta, \zeta} I_{\alpha z} I_{\beta \zeta} \left[\bar{G}_{\alpha\beta}^{(1)} \left(\frac{\Gamma_{\alpha z \parallel}}{n_{\alpha z}} - \frac{\Gamma_{\beta \zeta \parallel}}{n_{\beta \zeta}} \right) + \frac{\mu_{\alpha\beta}}{kT} \bar{G}_{\alpha\beta}^{(2)} \left(\frac{h_{\alpha z \parallel}}{\rho_{\alpha z}} - \frac{h_{\beta \zeta \parallel}}{\rho_{\beta \zeta}} \right) + \dots \right]$$

$$H_{\alpha z \parallel} \simeq \frac{kT}{m_{\alpha}} \sum_{\beta, \zeta} I_{\alpha z} I_{\beta \zeta} \left[\frac{5}{2} \frac{\mu_{\alpha\beta}}{m_{\alpha}} \bar{G}_{\alpha\beta}^{(2)} \left(\frac{\Gamma_{\alpha z \parallel}}{n_{\alpha z}} - \frac{\Gamma_{\beta \zeta \parallel}}{n_{\beta \zeta}} \right) + \bar{G}_{\alpha\beta}^{(4)} \frac{h_{\alpha z \parallel}}{p_{\alpha z}} - \bar{G}_{\alpha\beta}^{(5)} \frac{h_{\beta \zeta \parallel}}{p_{\beta \zeta}} + \dots \right]$$

with the driving 'forces' (created by the vertical drifts in a toroidal plasma)

$$-\nabla_{\parallel} p_{\alpha z} + z e n_{\alpha z} E_{\parallel} \quad \text{and} \quad -\frac{5}{2} \frac{p_{\alpha z}}{m_{\alpha}} \nabla_{\parallel} (kT)$$

3. constraints imposed by particle and energy balance equations

$$\frac{\Theta}{rR} \frac{\partial (R \Gamma_{\alpha z \parallel})}{\partial \theta} = \nabla_v \Gamma_{\alpha z, v}^{nc} + \dots \quad \text{and} \quad \frac{\Theta}{rR} \frac{\partial (R q_{\alpha z \parallel}^t)}{\partial \theta} = \nabla_v q_{\alpha z, v}^{nc} + \dots$$

$$q_{\alpha z \parallel}^t \simeq h_{\alpha z \parallel} + \frac{5}{2} kT \Gamma_{\alpha z \parallel}$$

relating the $\|\vec{B}$ fluxes to the radial pressure and temperature gradients as a function of the poloidal angle

without consideration of gyro-viscosity or anomalous viscosity effects the radial electric field drops out in the $\|\vec{B}$ flux-friction relations

Jül-3287
September 1996
ISSN 0944-2952