

# 1 Drift-kinetic classical transport

These notes derive the classical transport under the same set of assumptions as in the linearized drift-kinetic equation solved by the  $\delta f$ -code neoclassical code SFINCS (and probably most other neoclassical codes).

## 1.1 Motivation

For a mass-ratio expanded ion-impurity collision operator, we found that the classical transport of collisional impurities in W7-X can be comparable to the neoclassical transport. Thus, it would be of interest to have a general numerical tool to calculate the classical transport alongside the neoclassical transport from a drift-kinetic solver such as SFINCS.

## 1.2 Gyrophase dependent part of $f$

In many ways, calculating the classical transport is simpler than calculating the neoclassical transport, as the gyrophase dependent part of the distribution function is smaller than the gyrophase-independent in the expansion parameter  $\rho/L$ , and the gyrophase dependent part to required order is given entirely by the zeroth order gyrophase independent distribution. When  $f_{a0}$  is a Maxwellian  $f_{aM}$ , the gyrophase dependent part is given by

$$\tilde{f}_{a1} = -\vec{\rho}_a(\gamma) \cdot \nabla f_{Ma} = -\vec{\rho}(\gamma) \cdot \nabla \psi \frac{\partial f_{Ma}}{\partial \psi}, \quad (1)$$

where  $\gamma$  is the gyrophase,  $\psi$  a flux-label and  $\vec{\rho}$  the gyrophase vector

$$\vec{\rho}_a = \frac{1}{\Omega_a} \vec{b} \times \vec{v}_\perp, \quad (2)$$

with  $\vec{v}_\perp$  the velocity perpendicular to the magnetic field,  $\Omega_a = Z_a e B / m_a$  the gyrofrequency,  $\vec{b}$  the unit vector in the direction of the magnetic field  $\vec{B}$ ; and  $\psi$  a flux-label, which acts as our radial coordinate.

Equation 1 can be massaged a bit to yield (we drop the tilde since we will only consider the gyrophase dependent part of  $f_{a1}$  here)

$$f_{a1} = \frac{1}{\Omega_a} (\vec{b} \times \nabla \psi) \cdot \vec{v}_\perp \frac{\partial f_{Ma}}{\partial \psi}, \quad (3)$$

and we introduce the local coordinate system  $\vec{v}_\perp = v_2 \hat{e}_2 + v_3 \hat{e}_3$ , where  $\hat{e}_2, \hat{e}_3$  form an orthonormal triplet with  $\vec{b}$ . There is some freedom in how we align

our  $\hat{e}_2, \hat{e}_3$  coordinates, and we choose these vectors so that  $\hat{e}_2$  is entirely in the  $(\vec{b} \times \nabla\psi)$  direction. Thus

$$f_{a1} = \frac{1}{\Omega_a} |\vec{b} \times \nabla\psi| v_2 \frac{\partial f_{Ma}}{\partial \psi}. \quad (4)$$

Finally, we evaluate  $\frac{\partial f_{Ma}}{\partial \psi}$ . For heavy impurities, the lowest order distribution may vary on the flux-surface in response to a flux-surface variation of the electrostatic potential, in which case, we write

$$f_{Ma} = \eta_a(\psi) \left( \frac{m_a}{2\pi T_a} \right)^{3/2} \exp \left( -\frac{m_a v^2}{2T_a} - \frac{Z_a e \tilde{\Phi}}{T_a} \right), \quad (5)$$

where the *pseudo-density*  $\eta_a$  is related to the ordinary density by

$$\eta_a = n_a e^{Z_a e \tilde{\Phi}/T_a}. \quad (6)$$

The gradient thus becomes

$$\frac{\partial f_{Ma}}{\partial \psi} = f_{Ma} \left( \frac{d \ln \eta_a}{d \psi} + \frac{Z_a e}{T_a} \frac{\partial \tilde{\Phi}}{\partial \psi} + \frac{Z_a e \tilde{\Phi}}{T_a} \frac{d \ln T_a}{d \psi} + \left[ \frac{m_a v^2}{2T_a} - \frac{3}{2} \right] \frac{d \ln T_a}{d \psi} \right). \quad (7)$$

To simplify notation, we will introduce the quantities

$$\alpha_{1a} \equiv \frac{d \ln \eta_a}{d \psi} + \frac{Z_a e}{T_a} \frac{\partial \tilde{\Phi}}{\partial \psi} + \frac{Z_a e \tilde{\Phi}}{T_a} \frac{d \ln T_a}{d \psi} - \frac{3}{2} \frac{d \ln T_a}{d \psi} \quad (8)$$

$$\alpha_{2a} \equiv \frac{d \ln T_a}{d \psi}, \quad (9)$$

so that  $\frac{\partial f_{Ma}}{\partial \psi} = f_{Ma}(\alpha_{a1} + \alpha_{2a} x_a^2)$ , where

$$x_a^2 \equiv \frac{m_a v^2}{2T_a} \equiv \frac{v^2}{v_{Ta}^2}. \quad (10)$$

Thus

$$f_{a1} = \frac{|\vec{b} \times \nabla\psi|}{\Omega_a} v_2 f_{Ma} (\alpha_{1a} + \alpha_{2a} x_a^2). \quad (11)$$

### 1.3 Radial fluxes

The classical radial flux of particle and heat is given by

$$\Gamma_a \equiv \langle \vec{\Gamma}_a \cdot \nabla\psi \rangle^c \equiv \left\langle \frac{\vec{b} \times \nabla\psi}{Z_a e B} \cdot \vec{R}_a \right\rangle, \quad (12)$$

$$Q_a \equiv \langle \vec{Q}_a \cdot \nabla\psi \rangle^c \equiv \left\langle \frac{\vec{b} \times \nabla\psi}{Z_a e B} \cdot \vec{G}_a \right\rangle, \quad (13)$$

where we have introduced the *friction force* and *energy-weighted friction force*

$$\vec{R}_a = \int d^3v m_a \vec{v} C[f_a], \quad (14)$$

$$\vec{G}_a = \int d^3v \frac{m_a v^2}{2} m_a \vec{v} C[f_a]. \quad (15)$$

Here,  $C[f_a]$  is the Fokker-Planck collision operator accounting for the effects of all species acting on  $f_a$

$$C[f_a] = \sum_b C_{ab}[f_a, f_b]. \quad (16)$$

An important property of the Fokker-Planck operator is that it preserves the gyrophase dependence of  $f_a$ . Thus, only the gyrophase dependent part of  $f_a$  will contribute to the friction force in the  $\vec{b} \times \nabla\psi$  direction. As the gyrophase dependent part of  $f_a$  acts as a small correction to  $f_{Ma}$ , we can linearize the Fokker-Planck operator around  $f_{Ma}$  and write

$$\begin{aligned} C[f_a] &= \sum_b C_{ab}[f_{Ma} + f_{1a}, f_{Mb} + f_{1b}] \\ &\approx \sum_b C_{ab}[f_{Ma}, f_{Mb}] + C_{ab}[f_{Ma}, f_{b1}] + C_{ab}[f_{a1}, f_{Mb}], \end{aligned} \quad (17)$$

where the gyrophase-independent  $C_{ab}[f_{Ma}, f_{Mb}]$  part will not contribute to the classical transport. With this result, we write the relevant components of  $\vec{R}_a$  and  $\vec{G}_a$  as

$$\vec{b} \times \nabla\psi \cdot \vec{R}_a = m_a |\vec{b} \times \nabla\psi| \sum_b \int d^3v v_2 (C_{ab}[f_{a1}, f_{Mb}] + C_{ab}[f_{Ma}, f_{b1}]), \quad (18)$$

$$\vec{b} \times \nabla\psi \cdot \vec{G}_a = m_a T_a |\vec{b} \times \nabla\psi| \sum_b \int d^3v v_2 x_a^2 (C_{ab}[f_{a1}, f_{Mb}] + C_{ab}[f_{Ma}, f_{b1}]). \quad (19)$$

Inserting our expressions for  $f_1$ , we thus get

$$\begin{aligned} (\vec{b} \times \nabla\psi) \cdot \vec{R}_a &= m_a |\vec{b} \times \nabla\psi|^2 \sum_b \int d^3v v_2 \left( \frac{\alpha_{1a}}{\Omega_a} C_{ab}[v_2 f_{Ma}, f_{Mb}] + \frac{\alpha_{2a}}{\Omega_a} C_{ab}[v_2 x_a^2 f_{Ma}, f_{Mb}] \right. \\ &\quad \left. + \frac{\alpha_{1b}}{\Omega_b} C_{ab}[f_{Ma}, v_2 f_{Mb}] + \frac{\alpha_{2b}}{\Omega_b} C_{ab}[f_{Ma}, v_2 x_b^2 f_{Mb}] \right), \end{aligned} \quad (20)$$

$$\begin{aligned} (\vec{b} \times \nabla\psi) \cdot \vec{G}_a &= m_a T_a |\vec{b} \times \nabla\psi|^2 \sum_b \int d^3v v_2 x_a^2 \left( \frac{\alpha_{1a}}{\Omega_a} C_{ab}[v_2 f_{Ma}, f_{Mb}] + \frac{\alpha_{2a}}{\Omega_a} C_{ab}[v_2 x_a^2 f_{Ma}, f_{Mb}] \right. \\ &\quad \left. + \frac{\alpha_{1b}}{\Omega_b} C_{ab}[f_{Ma}, v_2 f_{Ma}] + \frac{\alpha_{2b}}{\Omega_b} C_{ab}[f_{Ma}, v_2 x_b^2 f_{Ma}] \right). \end{aligned} \quad (21)$$

These friction-force projections can be conveniently expressed in terms of Braginskii matrix elements

$$M_{ab}^{jk} = \frac{\tau_{ab}}{n_a} \int v_2 L_j^{(3/2)}(x_a^2) C_{ab} \left[ \frac{m_a v_2}{T_a} L_k^{(3/2)}(x_a^2) f_{a0}, f_{b0} \right] \quad (22)$$

$$N_{ab}^{jk} = \frac{\tau_{ab}}{n_a} \int v_2 L_j^{(3/2)}(x_a^2) C_{ab} \left[ f_{a0}, \frac{m_b v_2}{T_b} L_k^{(3/2)}(x_b^2) f_{b0} \right], \quad (23)$$

where

$$\tau_{ab} = \frac{12\pi^{3/2}\epsilon_0^2}{\sqrt{2}e^4 \ln \Lambda} \frac{m_a^{1/2} T_a^{3/2}}{Z_a^2 Z_b^2 n_b}, \quad (24)$$

and the relevant Sonine polynomials are

$$L_0^{(3/2)}(x_a^2) = 1 \quad (25)$$

$$L_1^{(3/2)}(x_a^2) = \frac{5}{2} - x_a^2, \quad (26)$$

so that

$$x_a^2 - \frac{5}{2} = -L_1^{(3/2)}(x_a^2) \quad (27)$$

$$x_a^2 = \frac{5}{2} L_0^{(3/2)}(x_a^2) - L_1^{(3/2)}(x_a^2) \quad (28)$$

$$1 = L_0^{(3/2)}(x_a^2). \quad (29)$$

Equation 27 makes it convenient to calculate the conductive heat flux  $q_a = Q_a - \frac{5}{2} T_a \Gamma_a$  rather than directly calculating  $Q_a$ . With this in mind, we write

$$\begin{aligned} (\vec{b} \times \nabla \psi) \cdot \vec{R}_a &= m_a |\vec{b} \times \nabla \psi|^2 \sum_b \frac{n_a}{\tau_{ab}} \left[ \frac{\alpha_{1a}}{\Omega_a} \frac{T_a}{m_a} M_{ab}^{00} + \frac{\alpha_{2a}}{\Omega_a} \frac{T_a}{m_a} \left( \frac{5}{2} M_{ab}^{00} - M_{ab}^{01} \right) \right. \\ &\quad \left. + \frac{\alpha_{1b}}{\Omega_b} \frac{T_b}{m_b} N_{ab}^{00} + \frac{\alpha_{2b}}{\Omega_b} \frac{T_b}{m_b} \left( \frac{5}{2} N_{ab}^{00} - N_{ab}^{01} \right) \right], \end{aligned} \quad (30)$$

$$\begin{aligned} (\vec{b} \times \nabla \psi) \cdot \left( \vec{G}_a - T_a \frac{5}{2} \vec{R}_a \right) &= -m_a T_a |\vec{b} \times \nabla \psi|^2 \sum_b \frac{n_a}{\tau_{ab}} \left[ \frac{\alpha_{1a}}{\Omega_a} \frac{T_a}{m_a} M_{ab}^{10} + \frac{\alpha_{2a}}{\Omega_a} \frac{T_a}{m_a} \left( \frac{5}{2} M_{ab}^{10} - M_{ab}^{11} \right) \right. \\ &\quad \left. + \frac{\alpha_{1b}}{\Omega_b} \frac{T_b}{m_b} N_{ab}^{10} + \frac{\alpha_{2b}}{\Omega_b} \frac{T_b}{m_b} \left( \frac{5}{2} N_{ab}^{10} - N_{ab}^{11} \right) \right]. \end{aligned} \quad (31)$$

The classical particle-flux and heat-flux thus become

$$\Gamma_a = \frac{m_a}{Z_a e^2} \left\langle |\nabla \psi|^2 \sum_b \frac{n_a n_b}{B^2 \tau_{ab} n_b} \left[ \frac{\alpha_{1a} T_a}{Z_a} M_{ab}^{00} + \frac{\alpha_{2a} T_a}{Z_a} \left( \frac{5}{2} M_{ab}^{00} - M_{ab}^{01} \right) + \frac{\alpha_{1b} T_b}{Z_b} N_{ab}^{00} + \frac{\alpha_{2b} T_b}{Z_b} \left( \frac{5}{2} N_{ab}^{00} - N_{ab}^{01} \right) \right] \right\rangle \quad (32)$$

$$q_a = - \frac{T_a m_a}{Z_a e^2} \left\langle |\nabla \psi|^2 \sum_b \frac{n_a n_b}{B^2 \tau_{ab} n_b} \left[ \frac{\alpha_{1a} T_a}{Z_a} M_{ab}^{10} + \frac{\alpha_{2a} T_a}{Z_a} \left( \frac{5}{2} M_{ab}^{10} - M_{ab}^{11} \right) + \frac{\alpha_{1b} T_b}{Z_b} N_{ab}^{10} + \frac{\alpha_{2b} T_b}{Z_b} \left( \frac{5}{2} N_{ab}^{10} - N_{ab}^{11} \right) \right] \right\rangle. \quad (33)$$

The values for the matrix-components can be found in the appendix of Helander+Sigmar. We can simplify the above expressions slightly by noting the symmetry properties

$$M_{ab}^{jk} = M_{ab}^{kj}, \quad (34)$$

$$N_{ab}^{jk} = \frac{T_a v_{Ta}}{T_b v_{Tb}} N_{ba}^{kj}, \quad (35)$$

$$N_{ab}^{j0} = -M_{ab}^{j0} = -M_{ab}^{0j}, \quad (36)$$

$$N_{ab}^{0j} = \frac{T_a v_{Ta}}{T_b v_{Tb}} N_{ba}^{j0} = -\frac{T_a v_{Ta}}{T_b v_{Tb}} M_{ba}^{j0} = -\frac{T_a^{3/2} m_b^{1/2}}{T_b^{3/2} m_a^{1/2}} M_{ba}^{0j}, \quad (37)$$

$$(38)$$

where the last property follows from applying the other 3. Thus, we only need

$$M_{ab}^{00} = - \frac{1 + \frac{m_a}{m_b}}{\left(1 + \frac{m_a T_b}{m_b T_a}\right)^{3/2}} = - \frac{\left(1 + \frac{m_a}{m_b}\right) \left(1 + \frac{m_a T_b}{m_b T_a}\right)}{\left(1 + \frac{m_a T_b}{m_b T_a}\right)^{5/2}} \quad (39)$$

$$M_{ab}^{01} = - \frac{3}{2} \frac{1 + \frac{m_a}{m_b}}{\left(1 + \frac{m_a T_b}{m_b T_a}\right)^{5/2}} \quad (40)$$

$$M_{ba}^{01} = - \frac{3}{2} \frac{1 + \frac{m_b}{m_a}}{\left(1 + \frac{m_b T_a}{m_a T_b}\right)^{5/2}} = - \frac{3 \left(1 + \frac{m_a}{m_b}\right) \frac{m_b}{m_a} \left(\frac{m_a T_b}{m_b T_a}\right)^{5/2}}{\left(1 + \frac{m_a T_b}{m_b T_a}\right)^{5/2}} \quad (41)$$

$$M_{ab}^{11} = - \frac{\frac{13}{4} + 4 \frac{m_a T_b}{m_b T_a} + \frac{15}{2} \left(\frac{m_a T_b}{m_b T_a}\right)^2}{\left(1 + \frac{m_a T_b}{m_b T_a}\right)^{5/2}} \quad (42)$$

$$N_{ab}^{11} = \frac{27}{4} \frac{\frac{m_a}{m_b}}{\left(1 + \frac{m_a T_b}{m_b T_a}\right)^{5/2}}. \quad (43)$$

$$(44)$$

The property  $N_{ab}^{j0} = -M_{ab}^{j0} = -M_{ab}^{0j}$  also means that the radial electric field does not contribute to the classical heat or particle flux.

Writing out the  $\alpha_1$  and  $\alpha_2$  and employing the relevant symmetry properties, we obtain the particle flux

$$\begin{aligned} \Gamma_a = \frac{m_a}{Z_a e^2} \sum_b \frac{1}{\tau_{ab} n_b} & \left[ \left\langle n_a n_b \frac{|\nabla \psi|^2}{B^2} \right\rangle M_{ab}^{00} \left( \frac{T_a}{Z_a} \frac{d \ln \eta_a}{d\psi} - \frac{T_b}{Z_b} \frac{d \ln \eta_b}{d\psi} \right) \right. \\ & + \left\langle n_a n_b \frac{|\nabla \psi|^2}{B^2} e \tilde{\Phi} \right\rangle M_{ab}^{00} \left( \frac{d \ln T_a}{d\psi} - \frac{d \ln T_b}{d\psi} \right) \\ & \left. + \left\langle n_a n_b \frac{|\nabla \psi|^2}{B^2} \right\rangle \left( (M_{ab}^{00} - M_{ab}^{01}) \frac{T_a}{Z_a} \frac{d \ln T_a}{d\psi} - \left( M_{ab}^{00} - \frac{m_a T_b}{m_b T_a} M_{ab}^{01} \right) \frac{T_b}{Z_b} \frac{d \ln T_b}{d\psi} \right) \right] \end{aligned} \quad (45)$$

and the heat-flux

$$\begin{aligned} q_a = -\frac{T_a m_a}{Z_a e^2} \sum_b \frac{1}{\tau_{ab} n_b} & \left[ \left\langle n_a n_b \frac{|\nabla \psi|^2}{B^2} \right\rangle M_{ab}^{01} \left( \frac{T_a}{Z_a} \frac{d \ln \eta_a}{d\psi} - \frac{T_b}{Z_b} \frac{d \ln \eta_b}{d\psi} \right) \right. \\ & + \left\langle n_a n_b \frac{|\nabla \psi|^2}{B^2} e \tilde{\Phi} \right\rangle M_{ab}^{01} \left( \frac{d \ln T_a}{d\psi} - \frac{d \ln T_b}{d\psi} \right) \\ & \left. + \left\langle n_a n_b \frac{|\nabla \psi|^2}{B^2} \right\rangle \left( (M_{ab}^{01} - M_{ab}^{11}) \frac{T_a}{Z_a} \frac{d \ln T_a}{d\psi} - (M_{ab}^{01} + N_{ab}^{11}) \frac{T_b}{Z_b} \frac{d \ln T_b}{d\psi} \right) \right] \end{aligned} \quad (46)$$

## 2 SFINCS implementation

SFINCS uses normalized quantities (denoted with a hat), where the normalized radial fluxes are defined in terms of the physical fluxes as

$$\hat{\Gamma}_a = \frac{\bar{R}}{\bar{n}\bar{v}} \frac{1}{Z_a e} \left\langle B^{-2} (\vec{B} \times \nabla \hat{\psi}) \cdot \vec{R}_a \right\rangle, \quad (47)$$

$$\hat{Q}_a = \frac{\bar{R}}{\bar{n}\bar{v}\bar{T}} \frac{1}{Z_a e} \left\langle B^{-2} (\vec{B} \times \nabla \hat{\psi}) \cdot \vec{G}_a \right\rangle, \quad (48)$$

where  $\hat{\psi} = \psi/(\bar{B}\hat{R}^2)$  is just a new choice of radial coordinate rather than a normalization – see the SFINCS manual for more details. We also define the dimensionless parameters  $\alpha = e\bar{\Phi}/\bar{T}$  and  $\Delta = \frac{\sqrt{2\bar{m}\bar{T}}}{e\bar{R}\bar{B}}$ , and the dimensionless collisionality  $\nu_n$

$$\bar{\nu} \equiv \frac{\sqrt{2}}{12\pi^{3/2}} \frac{\bar{n}e^4 \ln \Lambda}{\epsilon_0^2 \bar{m}^{1/2} \bar{T}^{3/2}} \quad (49)$$

$$\nu_n \equiv \bar{\nu} \frac{\bar{R}\sqrt{\bar{m}}}{\sqrt{2\bar{T}}} = \frac{1}{12\pi^{3/2}} \frac{\bar{n}\bar{R}e^4 \ln \Lambda}{\epsilon_0^2 \bar{T}^2}, \quad (50)$$

so that

$$\frac{1}{\tau_{ab}n_b} = \frac{Z_a^2 Z_b^2}{\hat{m}_a^{1/2} \hat{T}_a^{3/2}} \frac{\sqrt{2} \bar{T}^{1/2}}{\bar{n} \bar{R} \bar{m}^{1/2}} \nu_n = \frac{Z_a^2 Z_b^2}{\hat{m}_a^{1/2} \hat{T}_a^{3/2}} \frac{\sqrt{2} \bar{T}^{1/2} \bar{m}^{1/2} \bar{B}}{\bar{n} \bar{R} \bar{B} \bar{m}} \nu_n = \frac{Z_a^2 Z_b^2}{\hat{m}_a^{1/2} \hat{T}_a^{3/2}} \frac{e \bar{B}}{\bar{n} \bar{m}} \Delta \nu_n. \quad (51)$$

With this, the normalized particle and conductive heat-flux becomes

$$\begin{aligned} \hat{\Gamma}_a = \frac{\Delta^2 \nu_n}{2} \frac{Z_a \hat{m}_a^{1/2}}{\hat{T}_a^{3/2}} \sum_b Z_b^2 & \left[ \left\langle \hat{n}_a \hat{n}_b \frac{|\bar{R} \nabla \hat{\psi}|^2}{\hat{B}^2} \right\rangle M_{ab}^{00} \left( \frac{\hat{T}_a}{Z_a} \frac{d \ln \eta_a}{d \hat{\psi}} - \frac{\hat{T}_b}{Z_b} \frac{d \ln \eta_b}{d \hat{\psi}} \right) \right. \\ & + \left\langle \hat{n}_a \hat{n}_b \frac{|\bar{R} \nabla \hat{\psi}|^2}{\hat{B}^2} \hat{\Phi}_1 \right\rangle \alpha M_{ab}^{00} \left( \frac{d \ln T_a}{d \hat{\psi}} - \frac{d \ln T_b}{d \hat{\psi}} \right) \\ & \left. + \left\langle \hat{n}_a \hat{n}_b \frac{|\bar{R} \nabla \hat{\psi}|^2}{\hat{B}^2} \right\rangle \left( (M_{ab}^{00} - M_{ab}^{01}) \frac{\hat{T}_a}{Z_a} \frac{d \ln T_a}{d \hat{\psi}} - \left( M_{ab}^{00} - \frac{\hat{m}_a \hat{T}_b}{\hat{m}_b \hat{T}_a} M_{ab}^{01} \right) \frac{\hat{T}_b}{Z_b} \frac{d \ln T_b}{d \hat{\psi}} \right) \right] \quad (52) \end{aligned}$$

$$\begin{aligned} \hat{q}_a = -\frac{\Delta^2 \nu_n}{2} \frac{Z_a \hat{m}_a^{1/2}}{\hat{T}_a^{3/2}} \sum_b Z_b^2 & \left[ \left\langle \hat{n}_a \hat{n}_b \frac{|\bar{R} \nabla \hat{\psi}|^2}{\hat{B}^2} \right\rangle M_{ab}^{01} \left( \frac{\hat{T}_a}{Z_a} \frac{d \ln \eta_a}{d \hat{\psi}} - \frac{\hat{T}_b}{Z_b} \frac{d \ln \eta_b}{d \hat{\psi}} \right) \right. \\ & + \left\langle \hat{n}_a \hat{n}_b \frac{|\bar{R} \nabla \hat{\psi}|^2}{\hat{B}^2} \hat{\Phi}_1 \right\rangle \alpha M_{ab}^{01} \left( \frac{d \ln T_a}{d \hat{\psi}} - \frac{d \ln T_b}{d \hat{\psi}} \right) \\ & \left. + \left\langle \hat{n}_a \hat{n}_b \frac{|\bar{R} \nabla \hat{\psi}|^2}{\hat{B}^2} \right\rangle \left( (M_{ab}^{01} - M_{ab}^{11}) \frac{\hat{T}_a}{Z_a} \frac{d \ln T_a}{d \hat{\psi}} - (M_{ab}^{01} + N_{ab}^{11}) \frac{\hat{T}_b}{Z_b} \frac{d \ln T_b}{d \hat{\psi}} \right) \right]. \quad (53) \end{aligned}$$

Finally, using  $\hat{n}_a = \hat{\eta}_a e^{-Z_a \alpha \hat{\Phi}_1 / \hat{T}_a}$ , we get

$$\hat{n}_a \hat{n}_b = \hat{\eta}_a \hat{\eta}_b \exp \left( -\alpha \hat{\Phi}_1 \left[ \frac{Z_a}{\hat{T}_a} + \frac{Z_b}{\hat{T}_b} \right] \right), \quad (54)$$

where  $\hat{\eta}$  is the “density” in SFINCS, which is a flux-function. In the code, we define

$$G_{ab}^{(1)} = \left\langle \exp \left( -\alpha \hat{\Phi}_1 \left[ \frac{Z_a}{\hat{T}_a} + \frac{Z_b}{\hat{T}_b} \right] \right) \frac{|\bar{R} \nabla \hat{\psi}|^2}{\hat{B}^2} \right\rangle \quad (55)$$

$$G_{ab}^{(2)} = \left\langle \exp \left( -\alpha \hat{\Phi}_1 \left[ \frac{Z_a}{\hat{T}_a} + \frac{Z_b}{\hat{T}_b} \right] \right) \frac{|\bar{R} \nabla \hat{\psi}|^2}{\hat{B}^2} \hat{\Phi}_1 \right\rangle, \quad (56)$$

so that

$$\begin{aligned}\hat{\Gamma}_a = & \frac{\Delta^2 \nu_n}{2} \frac{Z_a \hat{m}_a^{1/2} \hat{\eta}_a}{\hat{T}_a^{3/2}} \sum_b Z_b^2 \hat{\eta}_b \left[ G_{ab}^{(1)} M_{ab}^{00} \left( \frac{\hat{T}_a}{Z_a} \frac{d \ln \eta_a}{d \hat{\psi}} - \frac{\hat{T}_b}{Z_b} \frac{d \ln \eta_b}{d \hat{\psi}} \right) \right. \\ & + G_{ab}^{(2)} \alpha M_{ab}^{00} \left( \frac{d \ln T_a}{d \hat{\psi}} - \frac{d \ln T_b}{d \hat{\psi}} \right) \\ & \left. + G_{ab}^{(1)} \left( (M_{ab}^{00} - M_{ab}^{01}) \frac{\hat{T}_a}{Z_a} \frac{d \ln T_a}{d \hat{\psi}} - \left( M_{ab}^{00} - \frac{\hat{m}_a \hat{T}_b}{\hat{m}_b \hat{T}_a} M_{ab}^{01} \right) \frac{\hat{T}_b}{Z_b} \frac{d \ln T_b}{d \hat{\psi}} \right) \right],\end{aligned}\tag{57}$$

$$\begin{aligned}\hat{q}_a = & -\frac{\Delta^2 \nu_n}{2} \frac{Z_a \hat{m}_a^{1/2} \hat{\eta}_a}{\hat{T}_a^{1/2}} \sum_b Z_b^2 \hat{\eta}_b \left[ G_{ab}^{(1)} M_{ab}^{01} \left( \frac{\hat{T}_a}{Z_a} \frac{d \ln \eta_a}{d \hat{\psi}} - \frac{\hat{T}_b}{Z_b} \frac{d \ln \eta_b}{d \hat{\psi}} \right) \right. \\ & + G_{ab}^{(2)} \alpha M_{ab}^{01} \left( \frac{d \ln T_a}{d \hat{\psi}} - \frac{d \ln T_b}{d \hat{\psi}} \right) \\ & \left. + G_{ab}^{(1)} \left( (M_{ab}^{01} - M_{ab}^{11}) \frac{\hat{T}_a}{Z_a} \frac{d \ln T_a}{d \hat{\psi}} - (M_{ab}^{01} + N_{ab}^{11}) \frac{\hat{T}_b}{Z_b} \frac{d \ln T_b}{d \hat{\psi}} \right) \right],\end{aligned}\tag{58}$$

and

$$\hat{Q}_a = \hat{q}_a + \frac{5}{2} \hat{T}_a \hat{\Gamma}_a.\tag{59}$$

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