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Evaluation of relativistic transport coefficients and the generalized Spitzer function in devices with 3D geometry and finite collisionality

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The relativistic generalization of the linearized drift kinetic equation solver NEO-2 is presented which is used for computation of neoclassical transport coefficients and the generalized Spitzer function in 3D toroidal fusion devices (tokamaks and stellarators). This upgrade allows computations of the Spitzer function playing the role of current drive efficiency in the whole experimentally relevant temperature range, from mild temperatures where finite plasma collisionality effects are important to high temperatures where relativistic effects should be taken into account. Within the Galerkin method used for problem discretization over energy relativistic effects are included into a set of matrices constant on a flux surface. Those matrices determine coefficients of a coupled set of integro-differential equations with a reduced dimension which is of the same form as in the non-relativistic case. For energy discretization of the linearized relativistic Coulomb collision operator it is presented in spherical momentum space variables in the symmetric integral form derived directly from Beliaev-Budker expressions. The cancellation problem pertinent to the fully analytical representation of Braams and Karney does not appear in this form. Examples of evaluation of relativistic transport coefficients and the Spitzer function are presented.

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I. INTRODUCTION

Radiofrequency current drive computations within the adjoint approach[1] reduce these computations to phase space integration of a quasilinear source term determined by the solution of a wave propagation problem (ray tracing in case of ECCD) weighted with the generalized Spitzer function which plays the role of current drive efficiency. For plasma temperatures relevant for a fusion reactor this function must be computed from the relativistic kinetic equation since resonant electrons responsible for current generation are usually supra-thermal such that relativistic effects become significant. Therefore, most current drive efficiency models presently used (see, e.g., Ref. 2) take these effects into account. At the same time, most of these models treat plasma collisionality in asymptotical limits where the dimensionality of the drift kinetic equation can be significantly reduced. Namely, these are the high collisionality limit where the generalized Spitzer function is reduced to a classical Spitzer function independent of the device geometry, and the low collisionality limit (long mean free path regime) where the dimensionality of the drift kinetic equation is reduced to 2D using bounce averaging. Although the last limit is well justified in most experimentally relevant cases, ECCD scenarii are possible where finite plasma collisionality effects are important, and, respectively, the generalized Spitzer function must be computed without simplifications of the kinetic equation. Such computations have been realized earlier with help of the drift kinetic equation solver NEO-2 in the non-relativistic limit. This limit is sufficient for studies of finite plasma collisionality effects which occur at mild plasma temperatures. At the same time, the relativistic extension of the NEO-2 model is required to cover the whole reactor relevant parameter range. Such an extension is presented in this paper. For this, the linearized relativistic Coulomb collision integral has been transformed here to spherical momentum space variables starting directly from the original Beliaev and Budker form[3]. In contrast to the general analytical representation of Braams and Karney[4] where the collision integral is reduced to 1D integrals, here a 2D integral form is retained which is simpler and numerically more stable since the numerical cancellation problem at low temperatures does not appear in this 2D form. Within the discretization scheme adopted in NEO-2, computational cost of this 2D form is not significant. It should be noted that the cancellation problem is avoided also in the potential representation of the collision integral by Braams and Karney if the potentials are obtained by directly solving pertinent equations[5] instead of using their analytical integral form.

The structure of the paper is as follows. In section II the discretization scheme adopted in NEO-2 and its generalization to the case of the relativistic drift kinetic equation is presented. In section III

2D integral expressions for the linearized Coulomb collision integral are derived and matrix elements of this integral required in NEO-2 are presented. In section IV examples of NEO-2 calculations of the generalized Spitzer function and neoclassical transport coefficients are presented for tokamak and stellarator geometry. A summary is given in section V.

II. COMPUTATION OF RELATIVISTIC NEOCLASSICAL TRANSPORT AND THE GENERALIZED SPITZER FUNCTION WITHIN THE NEO-2 CODE: DISCRETIZATION OF THE LINEARIZED DRIFT KINETIC EQUATION

The linearized drift kinetic equation solver NEO-2 evaluates the matrix of neoclassical transport coefficients D_{jk} which link thermodynamic forces A_k and fluxes I_j via the relation

$$I_j = -n_\alpha \sum_{k=1}^{3} D_{jk} A_k. \tag{1}$$

In the general case allowing for relativistic effects expressions for all three thermodynamic fluxes and for the forces A_2 and A_3 are formally the same with their non-relativistic expressions (see Ref. 6),

$$I_1 = \Gamma_\alpha, \quad I_2 = \frac{Q_\alpha}{T_\alpha}, \quad I_3 = n_\alpha \left\langle V_{\parallel\alpha} B \right\rangle, \qquad A_2 = \frac{1}{T_\alpha}\frac{\partial T_\alpha}{\partial r}, \quad A_3 = \frac{e_\alpha \langle E_\parallel B\rangle}{T_\alpha \langle B^2\rangle}, \tag{2}$$

where n_α, T_α, Γ_α, Q_α and $V_{\parallel\alpha}$ are α-species density, temperature, flux surface averaged radial particle and energy flux densities and parallel flow velocity, respectively, while the first thermodynamic force,

$$A_1 = \frac{1}{n_\alpha}\frac{\partial n_\alpha}{\partial r} - \frac{e_\alpha E_r}{T_\alpha} - \left(\frac{3}{2} + \mathcal{R}\right)\frac{1}{T_\alpha}\frac{\partial T_\alpha}{\partial r}, \tag{3}$$

includes a relativistic correction[7,8]

$$\mathcal{R} = \frac{\mu}{C_{MJ}}\frac{\mathrm{d}C_{MJ}}{\mathrm{d}\mu}, \qquad C_{MJ} = C_{MJ}(\mu) = \sqrt{\frac{\pi}{2\mu}}\frac{\mathrm{e}^{-\mu}}{K_2(\mu)}, \qquad \mu = \frac{m_\alpha c^2}{T_\alpha}. \tag{4}$$

Here, r is effective radius[6], E_r, $E_\parallel$, B, c, e_α, m_α are co-variant radial and parallel electric field components, magnetic field strength, speed of light, α-species charge and rest mass, respectively, $\langle \dots \rangle$ denotes a neoclassical flux surface average, and K_n are modified Bessel functions of the second kind. Relativistic transport coefficients,

$$D_{jk} = \frac{1}{n_\alpha}\left\langle \int \mathrm{d}^3 u \; q_j^\dagger f_M g_k \right\rangle, \tag{5}$$

and equations for the normalized distribution functions g_k,

$$\hat{L} f_M g_k = q_k f_M, \tag{6}$$

are formally the same with respective non-relativistic expressions in Ref. 6 up to the change of the velocity space variable $\mathbf{v}$ to the normalized momentum $\mathbf{u} = \mathbf{p}/m_\alpha$. Here, f_M is a relativistic Maxwellian normalized to the density, $\int \mathrm{d}^3 u f_M(u) = n_\alpha$,

$$f_M(u) = \frac{n_\alpha C_{MJ}(\mu)}{\pi^{3/2} v_{T\alpha}^3} \mathrm{e}^{\mu(1-\gamma)}, \qquad \gamma = \sqrt{1 + \frac{u^2}{c^2}}, \qquad v_{T\alpha} = \sqrt{\frac{2T_\alpha}{m_\alpha}}, \tag{7}$$

and q_k are relativistic driving terms linked to their non-relativistic form q_k^{NR} defined in Ref. 6,

$$q_1^{\mathrm{NR}}(\mathbf{v}) = -v_g^r, \qquad q_2^{\mathrm{NR}}(\mathbf{v}) = -\frac{m_\alpha v^2}{2T_\alpha} v_g^r, \qquad q_3^{\mathrm{NR}}(\mathbf{v}) = v_\parallel B, \tag{8}$$

where $v_g^r = v_g^r(\mathbf{v})$ is the radial component of the non-relativistic guiding center velocity, by

$$q_{1,3} = \frac{1}{\gamma} q_{1,3}^{\mathrm{NR}}(\mathbf{u}), \qquad q_2 = \frac{2}{\gamma(1+\gamma)} q_2^{\mathrm{NR}}(\mathbf{u}). \tag{9}$$

In case of negligible cross-field rotation, evolution operator $\hat{L}$ in (6) is of zero order in Larmor radius. It takes a short form in field aligned coordinates $(r, \vartheta, \varphi_0)$ where the unit vector along the magnetic field has only one non-zero contra-variant component $h^\vartheta = \mathbf{B} \cdot \nabla\vartheta / B$, and using zero order invariants of motion u and $\eta = u_\perp^2/(u^2 B)$ as momentum space variables,

$$\hat{L} = \frac{u \lambda h^\vartheta}{\gamma} \frac{\partial}{\partial \vartheta} - \hat{L}_C. \tag{10}$$

Here $\lambda \equiv u_\parallel / u = \cos\chi = \sigma\sqrt{1 - \eta B}$ is a pitch parameter (and χ is a pitch angle, respectively) with $\sigma = \pm 1$, and $\hat{L}_C$ is the linearized relativistic collision operator discussed in more details in the next section.

Kinetic equations (6) are solved by NEO-2 on a single long enough field line presenting normalized distributions g_k in the form of series expansion over some set of basis functions $\varphi_m(x)$,

$$g_k(\vartheta, u, \eta, \sigma) = \sum_{m'=0}^{M} g_{m'}^{(k)}(\vartheta, \eta, \sigma) \varphi_{m'}(x), \qquad x = \frac{u}{v_{T\alpha}}. \tag{11}$$

and projecting Eqs. (6) to the basis $\bar{\varphi}_m(x) = u\varphi_m(x)$ with help of integration of these equations weighted with $u^2 \bar{\varphi}_m(x)$ over the normalized momentum module u. Thus, each of 3D equations (6) is transformed to a set of coupled 2D integro-differential equations,

$$\lambda h^\vartheta \sum_{m'=0}^{M} \rho_{mm'} \frac{\partial g_m^{(k)}}{\partial \vartheta} - \kappa \sum_{m'=0}^{M} \left(\nu_{mm'} \hat{\mathcal{L}} g_{m'}^{(k)} + D_{mm'} g_{m'}^{(k)} + \sum_{l=0}^{L} I_{mm'}^l P_l(\lambda) \int_{-1}^{1} \mathrm{d}\lambda' P_l(\lambda') g_{m'}^{(k)} \right) = q_m^{(k)}, \tag{12}$$

where

$$\rho_{mm'} = \int\limits_0^\infty \mathrm{d}u u^3 f_M(u) \bar{\varphi}_m(x) \varphi_{m'}(x), \qquad q_m^{(k)}(\vartheta,\eta) = \int\limits_0^\infty \mathrm{d}u u^2 f_M(u) \bar{\varphi}_m(x) q_k(\vartheta,u,\eta), \tag{13}$$

and the second sum over m' comes from discretization of collision operator $\hat{L}_C$. There,

$$\mathcal{L} = 2\lambda \frac{\partial}{\partial \eta} \frac{\lambda \eta}{B} \frac{\partial}{\partial \eta} = \frac{1}{2} \frac{\partial}{\partial \lambda} \left(1-\lambda^2\right) \frac{\partial}{\partial \lambda} = \frac{1}{2 \sin\chi} \frac{\partial}{\partial \chi} \sin\chi \frac{\partial}{\partial \chi} \tag{14}$$

is the Lorentz operator, $P_l(\lambda)$ are Legendre polynomials ($L \to \infty$), and the rest are constant coefficients explicitly defined by Eqs. (46) - (48) in section III D. Equation set (12) corresponds here to the electron component treated in the infinite ion to electron mass ratio limit where this equation is decoupled from other components. This set is solved by NEO-2 using an adaptive finite volume discretization and iterative account of the integral part. This set is the same with the respective non-relativistic equation set[6] up to a definition of (constant on a flux surface) matrix elements $\rho_{mm'}$, $\nu_{mm'}$, $D_{mm'}$ and $I^l_{mm'}$ and source terms $q_m^{(k)}$ which differ from non-relativistic source terms by factors which are also constant on a flux surface and dependent only on the basis function index m.

III. LINEARIZED COULOMB COLLISION INTEGRAL

The relativistic form of the Coulomb collision integral[3] between test species a and field species b written in terms of normalized momenta $\mathbf{u} = \mathbf{p}/m_a$ and $\mathbf{u}' = \mathbf{p}'/m_b$ has the form[4]

$$\mathrm{St}(f_a, f_b) = \frac{\Gamma_{ab}}{2n_b} \int \mathrm{d}^3 u' \frac{\partial}{\partial \mathbf{u}} \cdot \mathbf{U} \cdot \left(f_b(\mathbf{u}') \frac{\partial f_a(\mathbf{u})}{\partial \mathbf{u}} - f_a(\mathbf{u}) \frac{m_a}{m_b} \frac{\partial f_b(\mathbf{u}')}{\partial \mathbf{u}'} \right), \tag{15}$$

where $\Gamma_{ab} = 4\pi e_a^2 e_b^2 n_b \Lambda_{ab} m_a^{-2}$ and tensor $\mathbf{U}$ is

$$\mathbf{U} = \frac{r^2}{\gamma \gamma' w^3} \left(w^2 \mathbf{I} - \mathbf{u}\mathbf{u} - \mathbf{u}'\mathbf{u}' + r\left(\mathbf{u}'\mathbf{u} + \mathbf{u}\mathbf{u}'\right)\right). \tag{16}$$

Here, $\mathbf{I}$ is a unit tensor, $\gamma = \left(1 + u^2/c^2\right)^{1/2}$ and $\gamma' = \left(1 + u'^2/c^2\right)^{1/2}$ are relativistic factors,

$$r = \gamma\gamma' - \frac{\mathbf{u}\cdot\mathbf{u}'}{c^2}, \qquad w = c\sqrt{r^2 - 1}, \tag{17}$$

where Λ_{ab} is the Coulomb logarithm. Linearization of the collision integral over perturbation δf_α with respect to the unperturbed Maxwellian $f_{M\alpha}$ such that $f_\alpha = f_{M\alpha} + \delta f_\alpha$ splits this integral into a differential and an integral part,

$$\mathrm{St}(f_a, f_b) \approx \hat{L}^{ab}_{CD} \delta f_a + \hat{L}^{ab}_{CI} \delta f_b, \qquad \hat{L}^{ab}_{CD} \delta f_a \equiv \mathrm{St}(\delta f_a, f_{Mb}), \qquad \hat{L}^{ab}_{CI} \delta f_b \equiv \mathrm{St}(f_{Ma}, \delta f_b). \tag{18}$$

A. Differential part

Using the isotropy of the Maxwellian, $f_{Mb} = f_{Mb}(u')$, and transforming the integration over d^3u' to spherical variables (u', α, β) with polar angle α counted from $\mathbf{u}$ direction, the differential part of the linearized collision operator is

$$\hat{L}^{ab}_{CD} = \frac{2\pi\Gamma_{ab}}{n_b}\frac{\partial}{\partial\mathbf{u}} \cdot \int\limits_0^\infty \mathrm{d}u' u'^2 \left(f_{Mb}\left(U_\perp \left(\mathbf{I} - \frac{\mathbf{uu}}{u^2}\right) + U_\parallel \frac{\mathbf{uu}}{u^2}\right) \cdot \frac{\partial}{\partial\mathbf{u}} - \frac{\partial f_{Mb}}{\partial u'} U \frac{\mathbf{u}}{u}\frac{m_a}{m_b}\right), \tag{19}$$

where functions $U_\perp = U_\perp(u, u')$, $U_\parallel = U_\parallel(u, u')$ and $U = U(u, u')$ result from averaging the tensor $\mathbf{U}$ over the angles, $\mathrm{d}^2\Omega' = \sin\alpha\, \mathrm{d}\alpha\, \mathrm{d}\beta$,

$$\frac{1}{4\pi}\int\limits_{4\pi} \mathrm{d}^2\Omega' \mathbf{U} = U_\parallel \frac{\mathbf{uu}}{u^2} + U_\perp \left(\mathbf{I} - \frac{\mathbf{uu}}{u^2}\right), \qquad \frac{1}{4\pi}\int\limits_{4\pi} \mathrm{d}^2\Omega' \mathbf{U} \cdot \frac{\mathbf{u}'}{u'} = U\frac{\mathbf{u}}{u}. \tag{20}$$

Explicitly these functions are the following integrals over variable $\xi = \cos\alpha$ such that $\mathbf{u}\cdot\mathbf{u}' = \xi u u'$,

$$U_\perp = \frac{1}{2\gamma\gamma'}\int\limits_{-1}^{1} \mathrm{d}\xi \frac{r^2}{w^3}\left(w^2 - \frac{1}{2}u'^2\left(1-\xi^2\right)\right),$$

$$U_\parallel = \frac{\gamma u'}{\gamma' u} U = \frac{\gamma u'^2}{2\gamma'}\int\limits_{-1}^{1} \mathrm{d}\xi \frac{r^2\left(1-\xi^2\right)}{w^3}. \tag{21}$$

Substituting in (19) the derivative of field Maxwellian,

$$\frac{\partial f_{Mb}}{\partial u'} = -\frac{m_b u'}{\gamma' T_b} f_{Mb}, \tag{22}$$

the most convenient form of operator (19) is obtained in spherical coordinates (u, χ, ϕ) where χ is the polar angle counted from the magnetic field direction (pitch angle) and ϕ is the gyrophase,

$$\hat{L}^{ab}_{CD} = \frac{1}{u^2}\frac{\partial}{\partial u} u^2 D^{uu}_{ab}\left(\frac{\partial}{\partial u} + \frac{m_a u}{\gamma T_b}\right) + \frac{1}{\sin\chi}\frac{\partial}{\partial\chi}\sin\chi D^{\chi\chi}_{ab}\frac{\partial}{\partial\chi} + \frac{1}{\sin^2\chi}\frac{\partial}{\partial\phi}D^{\chi\chi}_{ab}\frac{\partial}{\partial\phi}. \tag{23}$$

Here diffusion coefficients are

$$D^{uu}_{ab}(u) = \frac{2\pi\Gamma_{ab}}{n_b}\int\limits_0^\infty \mathrm{d}u' u'^2 f_{Mb}(u') U_\parallel, \qquad D^{\chi\chi}_{ab}(u) = \frac{2\pi\Gamma_{ab}}{n_b u^2}\int\limits_0^\infty \mathrm{d}u' u'^2 f_{Mb}(u') U_\perp. \tag{24}$$

B. Integral part

The integral part of collision integral (18) can be presented using integration by parts as

$$\hat{L}^{ab}_{CI}\delta f_b = \frac{\Gamma_{ab}}{2n_b}\int \mathrm{d}^3u' \delta f_b(\mathbf{u}')\Phi(\mathbf{u}, \mathbf{u}'), \tag{25}$$

where

$$\Phi(\mathbf{u},\mathbf{u}') = \frac{\partial}{\partial \mathbf{u}} \cdot \left(\mathbf{U} \cdot \frac{\partial f_{Ma}(u)}{\partial \mathbf{u}} + f_{Ma}(u) \frac{m_a}{m_b} \frac{\partial}{\partial \mathbf{u}'} \cdot \mathbf{U} \right) = \Phi(u, u', \xi) \tag{26}$$

and $\xi = \mathbf{u}\cdot\mathbf{u}'/(uu')$ is the same as introduced above. Last expression follows from the fact that scalar Φ depends on $\mathbf{u}$ and $\mathbf{u}'$ only via various scalar products of these two vectors. In the only practically important case of $\delta f_b(\mathbf{u}')$ independent of gyrophase ϕ' of spherical coordinates (u', χ', ϕ') function Φ can be replaced in (25) with its gyroaverage $\langle \Phi \rangle_{\phi'}$. Expanding Φ over Legendre polynomials,

$$\Phi = \sum_{l=0}^{\infty} \Phi_l(u,u') P_l(\xi), \qquad \Phi_l(u,u') = \frac{2l+1}{2} \int_{-1}^{1} \mathrm{d}\xi P_l(\xi) \Phi(u,u',\xi), \tag{27}$$

and using the spherical harmonics summation formula

$$P_l(\xi) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y^*_{lm}(\chi', \phi') Y_{lm}(\chi, \phi), \tag{28}$$

where spherical coordinates χ and ϕ pertain to $\mathbf{u}$, spherical harmonics are defined as follows,

$$Y_{lm}(\chi, \phi) = \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos\chi) \exp(im\phi), \tag{29}$$

and P_l^m are associated Legendre polynomials (in particular, $P_l^0 = P_l$), the gyroaverage $\langle \Phi \rangle_{\phi'}$ is

$$\langle \Phi \rangle_{\phi'} \equiv \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{d}\phi' \Phi = \sum_{l=0}^{\infty} \Phi_l(u,u') P_l(\cos\chi') P_l(\cos\chi). \tag{30}$$

Thus, Eq. (25) takes the form

$$\hat{L}^{ab}_{CI} \delta f_b = \frac{2\pi\Gamma_{ab}}{n_b} \sum_{l=0}^{\infty} \frac{P_l(\cos\chi)}{2l+1} \int_0^{\infty} \mathrm{d}u' u'^2 \Phi_l(u,u') \delta f_b^l(u') = \frac{\Gamma_{ab}}{2n_b} \sum_{l=0}^{\infty} P_l(\cos\chi) \int \mathrm{d}^3u' P_l(\xi)\, \Phi\, \delta f_b^l(u'), \tag{31}$$

where δf_b^l are Legendre series expansion coefficients of δf_b,

$$\delta f_b^l(u') = \frac{2l+1}{2} \int_0^{\pi} \mathrm{d}\chi' \sin\chi' P_l(\cos\chi') \delta f_b(u', \chi'). \tag{32}$$

Second equality (31) follows from integration in spherical variables (u', α, β) used above taking into account the second equation (27) and short notation $\xi = \cos\alpha$. Last integral in (31) can be transformed using integration by parts in vector form where $\xi = \xi(\mathbf{u},\mathbf{u}')$ and $\Phi = \Phi(\mathbf{u},\mathbf{u}')$,

$$\begin{aligned} \int \mathrm{d}^3u' P_l(\xi)\, \Phi\, \delta f_b^l(u') = {} & \frac{\partial}{\partial \mathbf{u}} \cdot \int \mathrm{d}^3u'\, \mathbf{U} \cdot \left(P_l(\xi)\, \delta f_b^l(u') \frac{\partial f_{Ma}(u)}{\partial \mathbf{u}} - f_{Ma}(u) \frac{m_a}{m_b} \frac{\partial}{\partial \mathbf{u}'} P_l(\xi)\, \delta f_b^l(u') \right) \\ & - \int \mathrm{d}^3u'\, \mathbf{U} : \left(P_l'(\xi)\, \delta f_b^l(u') \frac{\partial \xi}{\partial \mathbf{u}} \frac{\partial f_{Ma}(u)}{\partial \mathbf{u}} - f_{Ma}(u) \frac{m_a}{m_b} \frac{\partial}{\partial \mathbf{u}'} P_l'(\xi)\, \delta f_b^l(u') \frac{\partial \xi}{\partial \mathbf{u}} \right), \end{aligned} \tag{33}$$

where $P_l'(\xi)$ stands for the derivative of $P_l(\xi)$. First term here is a divergence of some vector $\mathbf{a}$ which can only be parallel to $\mathbf{u}$ so that

$$\frac{\partial}{\partial \mathbf{u}} \cdot \mathbf{a} = \frac{1}{u^2}\frac{\partial}{\partial u} u\, \mathbf{u} \cdot \mathbf{a}. \tag{34}$$

Using this relation and the normalized perturbed distribution function $g_b = \delta f_b / f_{Mb}$ such that $\delta f_b^l = g_b^l f_{Mb}$, Eq. (33) is transformed to

$$\begin{aligned}
\frac{m_b}{m_a}\int \mathrm{d}^3u' P_l(\xi)\, \Phi\, f_l(u') = &-\frac{1}{u^2}\frac{\partial}{\partial u} u f_{Ma}(u) \int \mathrm{d}^3u'\ f_{Mb}(u')\ \mathbf{u}\cdot\mathbf{U}\cdot\frac{\partial}{\partial \mathbf{u'}} P_l(\xi)\, g_b^l(u') \\
&+ f_{Ma}(u)\int \mathrm{d}^3u'\ f_{Mb}(u')\ \mathbf{U} : \frac{\partial}{\partial \mathbf{u'}} P_l'(\xi)\, g_b^l(u') \frac{\partial \xi}{\partial \mathbf{u}} \\
&+ \left(1 - \frac{T_b}{T_a}\right)\frac{1}{u^2}\frac{\partial}{\partial u} f_{Ma}(u) \frac{m_b u}{\gamma T_b}\int \mathrm{d}^3u'\ f_{Mb}(u')\ \mathbf{u}\cdot\mathbf{U}\cdot\mathbf{u}\, P_l(\xi)\, g_b^l(u') \\
&- \left(1 - \frac{T_b}{T_a}\right) f_{Ma}(u) \frac{m_b}{\gamma T_b}\int \mathrm{d}^3u'\ f_{Mb}(u')\ \mathbf{u}\cdot\mathbf{U}\cdot\frac{\partial \xi}{\partial \mathbf{u}} P_l'(\xi)\, g_b^l(u'),
\end{aligned} \tag{35}$$

where derivatives of Maxwellians have been substituted explicitly and relations $\gamma' \mathbf{u}\cdot\mathbf{U}\cdot\mathbf{u} = \gamma \mathbf{u'}\cdot\mathbf{U}\cdot\mathbf{u}$ and $\gamma' \mathbf{u}\cdot\mathbf{U}\cdot\partial\xi/\partial\mathbf{u} = \gamma \mathbf{u'}\cdot\mathbf{U}\cdot\partial\xi/\partial\mathbf{u}$ have been used. Since subintegrands in (35) are independent of azimuth β, integration in spherical variables is reduced to 2D resulting for the integral part (31) in

$$\begin{aligned}
\hat{L}_{CI}^{ab} g_b f_{Mb} = &\frac{\pi m_a \Gamma_{ab}}{m_b n_b}\sum_{l=0}^{\infty} P_l(\cos\chi)\left[f_{Ma}(u)\int_0^\infty \mathrm{d}u' u'^2 f_{Mb}(u')\left(R_{00}^{(l)}(u,u') g_b^l(u') + R_{01}^{(l)}(u,u')\frac{\partial g_b^l(u')}{\partial u'}\right)\right. \\
&\left. - \frac{1}{u^2}\frac{\partial}{\partial u} u^2 f_{Ma}(u) \int_0^\infty \mathrm{d}u' u'^2 f_{Mb}(u')\left(R_{10}^{(l)}(u,u') g_b^l(u') + R_{11}^{(l)}(u,u')\frac{\partial g_b^l(u')}{\partial u'}\right)\right] \\
&+ \frac{\pi m_a \Gamma_{ab}}{T_b n_b}\left(\frac{T_b}{T_a} - 1\right)\sum_{l=0}^{\infty} P_l(\cos\chi)\left[f_{Ma}(u)\int_0^\infty \mathrm{d}u' u'^2 f_{Mb}(u')\frac{u'}{\gamma'} R_{01}^{(l)}(u,u') g_b^l(u')\right. \\
&\left. - \frac{1}{u^2}\frac{\partial}{\partial u} u^2 f_{Ma}(u) \int_0^\infty \mathrm{d}u' u'^2 f_{Mb}(u')\frac{u'}{\gamma'} R_{11}^{(l)}(u,u') g_b^l(u'),\right],
\end{aligned} \tag{36}$$

where

$$R_{00}^{(l)}(u,u') = \int_{-1}^{1} \mathrm{d}\xi \left(P_l'(\xi)\, \mathbf{U} : \frac{\partial^2 \xi}{\partial \mathbf{u} \partial \mathbf{u}'} + P_l''(\xi)\, \frac{\partial \xi}{\partial \mathbf{u}} \cdot \mathbf{U} \cdot \frac{\partial \xi}{\partial \mathbf{u}'} \right),$$

$$R_{01}^{(l)}(u,u') = \int_{-1}^{1} \mathrm{d}\xi P_l'(\xi)\, \frac{\partial \xi}{\partial \mathbf{u}} \cdot \mathbf{U} \cdot \frac{\mathbf{u}'}{u'},$$

$$R_{10}^{(l)}(u,u') = \int_{-1}^{1} \mathrm{d}\xi P_l'(\xi)\, \frac{\mathbf{u}}{u} \cdot \mathbf{U} \cdot \frac{\partial \xi}{\partial \mathbf{u}'},$$

$$R_{11}^{(l)}(u,u') = \int_{-1}^{1} \mathrm{d}\xi P_l(\xi)\, \frac{\mathbf{u}}{u} \cdot \mathbf{U} \cdot \frac{\mathbf{u}'}{u'}, \tag{37}$$

are symmetric kernels,

$$R_{kk'}^{(l)}(u,u') = R_{k'k}^{(l)}(u',u), \tag{38}$$

and $P_l''(\xi)$ denotes a second derivative. Evaluating explicitly tensor convolutions in (37) and eliminating $P_l''(\xi)$ with help of the Legendre equation a compact explicit form of kernels (37) is obtained in dimensionless variables $z = u/c$ and $z' = u'/c$,

$$R_{kk'}^{(l)}(u,u') = c^{k+k'-3} \mathcal{R}_{kk'}^{(l)}(z,z'), \tag{39}$$

where dimensionless functions $\mathcal{R}_{kk'}^{(l)}$ are

$$\mathcal{R}_{00}^{(l)}(z,z') = \frac{1}{zz'\gamma\gamma'} \int_{-1}^{1} \frac{\mathrm{d}\xi}{\sqrt{r^2-1}} \left(1-\xi^2\right) r \left[r l(l+1) P_l'(\xi) + 2zz' \left(\xi P_l'(\xi) - l(l+1) P_l(\xi) \right) \right],$$

$$\mathcal{R}_{10}^{(l)}(z,z') = \frac{1}{z'} \int_{-1}^{1} \frac{\mathrm{d}\xi}{\sqrt{r^2-1}} \left[r \left(\frac{\gamma z'}{\gamma' z} - \xi \right) l(l+1) P_l(\xi) + \left(r + zz' \left(\frac{\gamma z'}{\gamma' z} - \xi \right) \right) \left(1-\xi^2\right) P_l'(\xi) \right],$$

$$\mathcal{R}_{11}^{(l)}(z,z') = \int_{-1}^{1} \frac{\mathrm{d}\xi}{\sqrt{r^2-1}} \left[\left(2r\xi + zz' \left(1-\xi^2\right) \right) P_l(\xi) - r \left(1-\xi^2\right) P_l'(\xi) \right], \tag{40}$$

where $r = \gamma\gamma' - zz'\xi$ and relativistic factors are $\gamma = \sqrt{1+z^2}$ and $\gamma' = \sqrt{1+z'^2}$.

C. Relation to Braams and Karney form

Integrals (21) and (40) can be computed analytically leading for diffusion coefficients (24) and for the integral kernels to Braams and Karney expressions. In particular, expressing results of integration of Eqs. (21) in terms of functions $j_*(z)$ defined in Ref. 4,

$$U_\perp = \frac{\gamma}{u\gamma'}\left(j'_{0[1]2} - 2\left(\frac{c^2}{u^2}+\frac{1}{\gamma^2}\right)j'_{0[2]02} + \frac{8c^2}{\gamma^2 u^2}j'_{0[3]022}\right), \qquad u' < u,$$

$$U_\perp = \frac{\gamma}{u'\gamma'}\left(\frac{\gamma'^2}{\gamma^2}j_{0[1]2} - 2\frac{u'^2}{u^2}\left(\frac{c^2}{u'^2}+\frac{1}{\gamma^2}\right)j_{0[2]02} + \frac{8c^2}{\gamma^2 u^2}j_{0[3]022}\right), \qquad u' > u, \tag{41}$$

$$U_\parallel = \frac{4\gamma c^2}{u^3\gamma'}\left(\gamma^2 j'_{0[2]02} - 4j'_{0[3]022}\right), \qquad u' < u,$$

$$U_\parallel = \frac{4\gamma c^2}{u^2 u'\gamma'}\left(\gamma'^2 j_{0[2]02} - 4j_{0[3]022}\right), \qquad u' > u, \tag{42}$$

where $j_* = j_*(z)$ and $j'_* = j_*(z')$, coefficients (24) coincide with the ones defined by Eqs.(34) of Ref. 4 up to re-notation $D^{uu}_{ab} = D^{s/s'}_{uu,0}$ and $D^{\chi\chi}_{ab} = D^{s/s'}_{\theta\theta,0}/u^2$. There is a known numerical cancellation problem which arises when analytical expressions are used directly at small temperatures where $z, z' \ll 1$. This problem is not severe for diffusion coefficients where it does not appear for double precision arithmetics and temperatures relevant for fusion devices (higher than few eV). Therefore, the Braams and Karney form is used in NEO-2 for evaluation of matrix elements of the operator $\hat{L}^{ab}_{CD}$. In turn, the cancellation problem becomes increasingly significant with increasing Legendre expansion order l in analytical expressions for integral kernels (40) where terms of the order $(zz')^{-l-1} \gg 1$ cancel. This problem does not appear if integrals (40) are computed numerically using $\sqrt{r-1}$ as a new integration variable. In NEO-2 these integrals are efficiently evaluated up to computer accuracy using high order quadrature formulas.

D. Matrix elements

For the electrons being of interest here collisions with (non-relativistic) ions are treated in the infinite ion mass limit where the ion distribution function is assumed to be known. In this limit, quantities (21) are $U_\perp = \gamma/u$ and $U_\parallel = 0$, and diffusion coefficients (24) are respectively reduced to a Lorentz limit,

$$D^{uu}_{ei} = 0, \qquad D^{\chi\chi}_{ei} = \frac{\Gamma_{ei}\gamma}{2u^3}. \tag{43}$$

The only non-vanishing kernels (39) in the electron-ion collision term are $\mathcal{R}^{(1)}_{00}(z,z') = 8\gamma/\left(3z^2 z'\right)$ and $\mathcal{R}^{(1)}_{01}(z,z') = 4\gamma/\left(3z^2\right)$ resulting for the integral part (36) in a simple expression via parallel ion flow velocity $V_{\parallel i}$,

$$\hat{L}^{ei}_{CI} g_i f_{Mi} = \frac{m_e \Gamma_{ei} V_{\parallel i}\gamma\lambda}{T_e u^2} f_{Me} \equiv q_4 f_{Me}, \qquad V_{\parallel i} = \frac{1}{n_i}\int \mathrm{d}^3u' u'\lambda' g_i f_{Mi}. \tag{44}$$

This integral part formally is an additional source in (6) while the only contribution of ions to the matrix elements of the total collision operator $\hat{L}_C = \hat{L}_{CD} + \hat{L}_{CI}$ is via the pitch-angle scattering coefficient (43),

$$\hat{L}_{CD} g_e f_{Me} = \left(\hat{L}_{CD}^{ee} + \hat{L}_{CD}^{ei}\right) g_e f_{Me} = \frac{1}{u^2}\frac{\partial}{\partial u} u^2 D_{ee}^{uu} f_{Me} \frac{\partial g_e}{\partial u} + 2\left(D_{ee}^{\chi\chi} + D_{ei}^{\chi\chi}\right) f_{Me} \hat{\mathcal{L}} g_e, \tag{45}$$

as follows for gyrophase independent g_e from (23) and (14). Thus, matrix elements of the differential part of the collision operator in Eq. (12) for continuous basis functions $\varphi_m(x)$ are

$$\begin{aligned} \nu_{mm'} &= \frac{2}{\kappa}\int\limits_0^\infty \mathrm{d}u u^2 f_{Me}(u)\left(D_{ee}^{\chi\chi}(u) + D_{ei}^{\chi\chi}(u)\right)\bar{\varphi}_m(x)\varphi_{m'}(x), \\ D_{mm'} &= \frac{1}{\kappa}\int\limits_0^\infty \mathrm{d}u u^2 f_{Me}(u) D_{ee}^{uu}(u)\frac{\partial\bar{\varphi}_m(x)}{\partial u}\frac{\partial\varphi_{m'}(x)}{\partial u}, \end{aligned} \tag{46}$$

where

$$\kappa = \frac{4\Gamma_{ee}}{3\sqrt{\pi} v_{Te}^4} \tag{47}$$

is the inverse mean free path. The integral part of the collision operator in Eq. (12) is determined by electrons alone, $\hat{L}_{CI} = \hat{L}_{CI}^{ee}$. Matrix elements of this part follow from its definition (36),

$$\begin{aligned} I_{mm'}^l = \frac{6\pi^{3/2}}{2l+1}\frac{T_e^2}{n_e m_e}\int\limits_0^\infty \mathrm{d}u u^2 f_{Me}(u)\int\limits_0^\infty \mathrm{d}u' u'^2 f_{Me}(u')\Bigg(R_{00}^{(l)}(u,u')\bar{\varphi}_m(x)\varphi_{m'}(x') \\ + R_{01}^{(l)}(u,u')\bar{\varphi}_m(x)\frac{\partial\varphi_{m'}(x')}{\partial u'} + R_{10}^{(l)}(u,u')\frac{\partial\bar{\varphi}_m(x)}{\partial u}\varphi_{m'}(x') + R_{11}^{(l)}(u,u')\frac{\partial\bar{\varphi}_m(x)}{\partial u}\frac{\partial\varphi_{m'}(x')}{\partial u'}\Bigg), \end{aligned} \tag{48}$$

where $x = u/v_{Te}$ and $x' = u'/v_{Te}$.

It can be seen that matrix elements (46) and (48) are symmetric with respect to permutation of indices m and m' in case the projection basis $\bar{\varphi}_m$ is the same as test basis φ_m (see also Eq. (38)). In this case the collision operator in Eq. (12) would be automatically self-adjoint for any small number of basis functions. Due to the actual difference of projection and test basis, $\bar{\varphi}_m = u\varphi_m$, this property is not automatic in NEO-2 where Onsager symmetry of transport coefficients (5), which follows from self-adjointness of the collision operator, is used as a convergence measure.

In the non-relativistic limit, matrix elements (46) and (48) are independent of plasma parameters what can be seen if equation set (12) is multiplied with the matrix inverse to $\rho_{mm'}$, Eq. (13). This property is not hold anymore in the general case where dependence on temperature is essential.

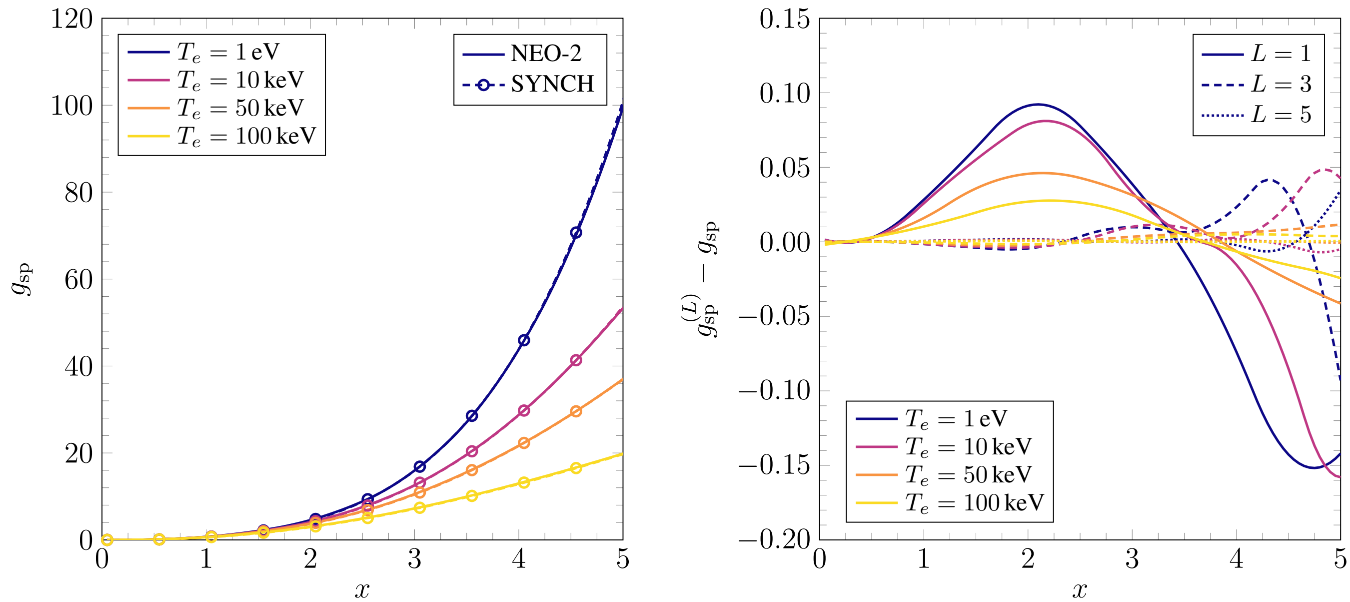

FIG. 1. Generalized Spitzer function g_{sp} from NEO-2 (solid) and SYNCH (dashed) (left) and error in this function, $g_{sp}^{(L)} - g_{sp}$, introduced by finite Legendre series representation of the collision operator (right) as functions of dimensionless momentum $x = u/v_{Te}$ for fixed pitch parameter $\lambda = 1$ and various temperatures. Results for g_{sp} from NEO-2 and SYNCH are shown with solid and dashed lines, respectively. Numbers of Legendre polynomials L used in the right plot for representation of the integral part of the collision operator for truncated solutions $g_{sp}^{(L)}$ are shown in the legend. Converged solutions g_{sp} from NEO-2 correspond to $L = 7$.

IV. BENCHMARK

One of the main outputs of NEO-2 is the generalized Spitzer function g_{sp} used for the computation of current drive efficiency within the adjoint approach. This function is the normalized solution of the conductivity problem determined by Eq. (6) with $k = 3$,

$$g_{sp} = \frac{3\sqrt{\pi}\kappa}{4B_{ref}} g_3, \tag{49}$$

where B_{ref} is a reference magnetic field (magnetic field module B averaged over Boozer angles). This normalization relates g_{sp} in the homogeneous magnetic field to the usual Spitzer function as follows $g_{sp} = \lambda D/A$ where D/A is tabulated for non-relativistic case in Ref. 9. Results of NEO-2 computations of the generalized Spitzer function in a tokamak with circular cross section are presented in Figs. 1 and 2. These results correspond to a magnetic field minimum point on the flux surface with aspect ratio $A = 7.9$ and rather low plasma collisionality, $2\pi R_0 \kappa = 10^{-3}$ where R_0 is a reference major

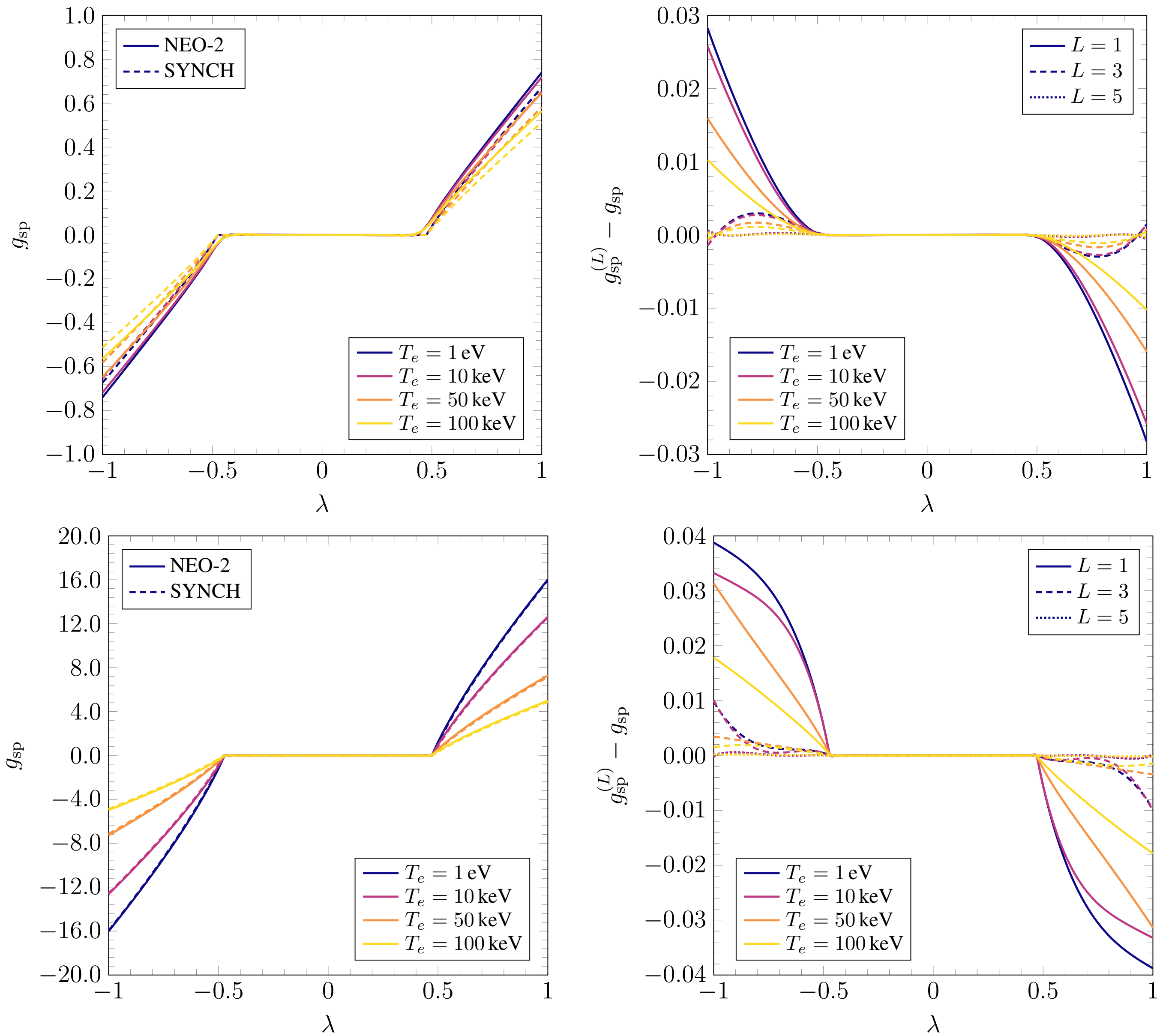

FIG. 2. The same quantities as in Fig. 1 as functions of pitch parameter λ for fixed dimensionless momentum $x = u/v_{Te}$ ($x = 1$ for upper row and $x = 3$ for lower row).

plasma radius and κ is the inverse mean free path (47). For comparison, the results of the solution of the bounce-averaged equation by the code SYNCH[10] are also shown. The latter code takes into account only a single, momentum conserving $l = 1$ term in the expansion (36) of the integral part of the collision operator over Legendre polynomials. It can be seen that this approximation is sufficient to reach an agreement with the exact model within a few percent in the thermal velocity space region (for $x = u/v_{Te} = 1$ relative error is about 5%, see Fig. 2, and this relative error decreases in the supra-thermal region because absolute error stays there the same as in the thermal region while the Spitzer function increases, see Fig. 1).

The effect of higher order Legendre polynomials in the integral part of the collision operator on neoclassical transport coefficients (5) is also limited to few percent, see Fig. 3 where these coefficients are presented for the same tokamak configuration as in Figs. 1 and 2. In this figure, (Onsager symmetric) electron transport coefficients $D_{ij} = D_{ji}$ normalized by their non-relativistic values for the same temperature are shown as functions of electron temperature. It can be seen that relativistic effects lead to higher values of axisymmetric particle and heat diffusion coefficients (coefficients which scale linearly with collision frequency) as compared to their non-relativistic values, see left plot of Fig. 3, what is in contrast to the well known reduction by relativistic effects of the conductivity coefficient D_{33} (scales inversely with collision frequency). It can also be seen that bootstrap/Ware pinch coefficient $D_{13} = D_{31}$ is practically unchanged by relativistic effects. Such a behavior is similar to D_{13} for a plasma component with only like-particle collisions taken into account. In this case D_{13} can be shown to be independent of relativistic effects.

The trend shown in Fig. 3 for axisymmetric particle and heat diffusivity coefficients D_{ij} with $i, j = 1, 2$ is different for the non-axisymmetric coefficients, see Fig. 4. In this figure, transport coefficients for the standard configuration of the Wendelstein 7-X stellarator are shown for the low collisional $1/\nu$-regime (collisionality $2\pi R\kappa = 10^{-3}$) at the flux surface $s = 0.25$ where s is the normalized toroidal flux. It can be seen that in contrast to a tokamak the relativistic effect on particle and heat diffusion coefficients is very weak (about 5% in the temperature range up to 100 keV as compared to 100% in the same range in a tokamak). This weak dependence has been shown earlier in Ref. 7 where these coefficients have been computed for the relativistic Lorentz model on the basis of the analytical approach of Ref. 11 for the non-relativistic case (for the Lorentz model, relativistic particle and heat diffusion coefficients normalized by their non-relativistic counter-parts are independent of the device geometry). It can be seen from Fig. 4 that the result of Ref. 7 is accurately reproduced by direct solution of the kinetic equation with the Lorentz collision model using NEO-2 (dashed lines in the left plot), and that the account of the full linearized collision operator (solid lines) does not introduce a principal difference in temperature dependencies but only adds a small (of the order of field modulation within the flux surface, which is about 9%), almost independent of the temperature correction due to energy scattering. As seen from the right plot of Fig. 4, relativistic trends for conductivity and bootstrap/Ware pinch coefficients are not different from those in a tokamak.

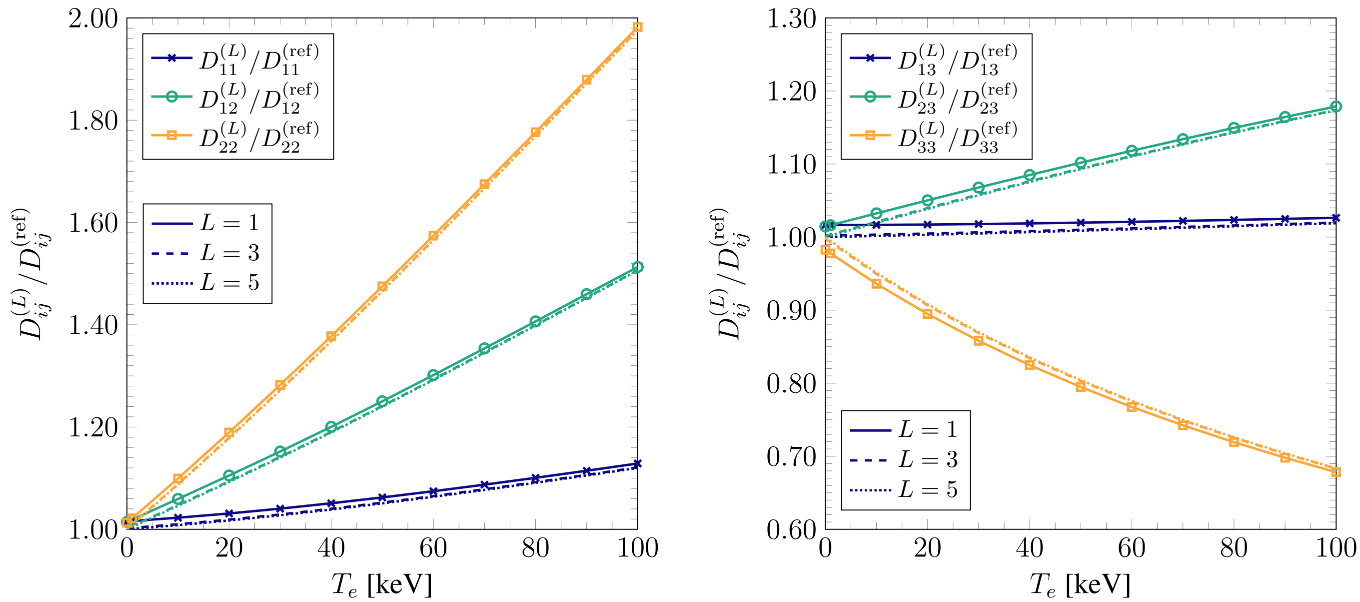

FIG. 3. Transport coefficients for electrons in a tokamak as functions of electron temperature T_e computed with various number of Legendre polynomials L in the expansion of the integral part of collision operator (see the legend). Each coefficient $D_{ij}^{(L)}$ is normalized by its reference value $D_{ij}^{(\mathrm{ref})}$ which corresponds to $L = 7$ expansion in non-relativistic limit. Since the curves corresponding to higher Legendre harmonics (dashed and dotted lines) are almost on top of each other, the markers for these curves have been omitted for reasons of clarity.

V. CONCLUSION

The drift kinetic equation solver NEO-2 for three dimensional geometries has been upgraded to use the relativistic Coulomb collision operator. For this upgrade, a compact representation of the full linearized relativistic Coulomb collision operator has been derived directly from the general Beliaev-Budker expression[3]. In this representation, kernels of the integral part of the collision operator are kept in the form of 1D integrals which are evaluated numerically in NEO-2. This is numerically more stable than the final fully analytical form of Braams and Karney[4] evaluated directly without using the recurrence relation. Benchmarking of NEO-2 in the long mean free path regime against the fully relativistic bounce averaged code SYNCH[10] shows an agreement in computations of the generalized Spitzer function within a few percent. The remaining difference is due to the truncation in SYNCH of the Legendre polynomial expansion of the integral part of the collision operator which takes into account only a single, first order Legendre polynomial responsible for the momentum

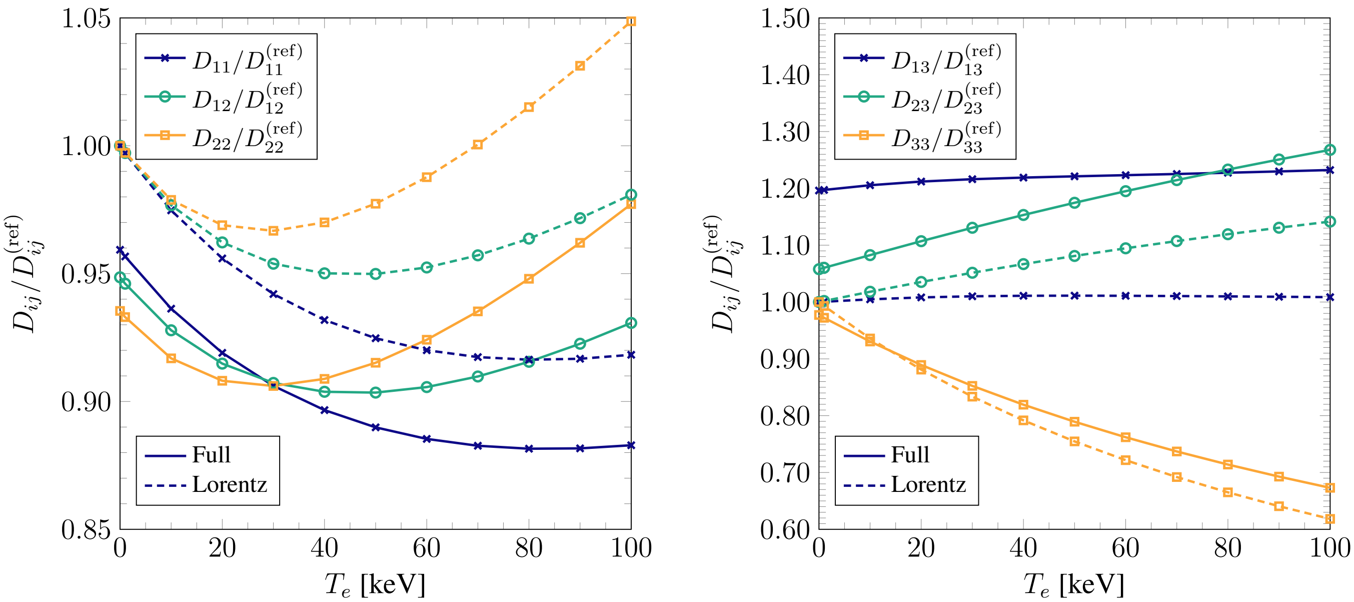

FIG. 4. Transport coefficients for electrons in a stellarator as functions of electron temperature T_e computed with full collision operator (solid) and Lorentz collision model (dashed), see the legend. Each coefficient D_{ij} is normalized by its reference value $D_{ij}^{(\mathrm{ref})}$ which corresponds to Lorentz model in non-relativistic limit.

conservation. Contributions of higher order Legendre polynomials remain limited to a few percent also in computations of neoclassical transport coefficients.

Changes produced by relativistic effects in axisymmetric neoclassical transport coefficients of electrons lead to the increase of most transport coefficients as compared to their non-relativistic values what is the opposite trend to the reduction of the conductivity coefficient which is the only coefficient reduced by the relativistic effects. The largest increase is in the heat diffusion coefficient D_{22} which scales with temperature roughly as $T_e/(100\,\mathrm{keV})$ and the least affected coefficient is bootstrap/Ware pinch coefficient $D_{31} = D_{13}$ whose relativistic change is about 1% at 100 keV. (It can be shown that the latter change is even completely absent in a single component plasma without inter-species collisions.)

Computations of non-axisymmetric transport coefficients in the $1/\nu$ regime have confirmed the result of Ref. 7 showing a rather small change of particle and heat diffusion coefficients by relativistic effects what is in contrast to axisymmetric coefficients. Namely, the semi-analytical result of Ref. 7 for the Lorentz collision model has been accurately reproduced by NEO-2. Full account of collisions does not introduce qualitative changes in this result but just slightly corrects it by a number of the order of the parallel field modulation amplitude. This is a usual correction due to scattering over energy.

With the present upgrade, NEO-2 is capable to model current drive efficiency in tokamaks and stellarators in the whole temperature range taking into account both, finite plasma collisionality important at low and mild plasma temperatures where relativistic effects are relatively small[12] as well as relativistic effects important at fusion reactor relevant temperatures. Thus, modelling of ECCD in stellarator geometries using a combination of the ray-tracing code TRAVIS[13] and NEO-2 can be continued without temperature limitation needed earlier.

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