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Computation of neoclassical transport coefficients and generalized Spitzer function in toroidal fusion plasmas

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Abstract

Neoclassical transport plays a significant role in toroidal magnetic confinement systems. In this work a detailed calculation of the moments of the full linearized Coulomb collision operator (collision matrix elements) in terms of test functions proportional to the associated Laguerre polynomials has been presented. These matrix elements have been implemented in the drift kinetic equation (DKE) solver NEO-2 (which is based on the field line integration technique) direct at the level of the DKE. Therefore, the NEO-2 code can calculate the complete (including energy diffusion and momentum recovery) local solution along the magnetic field line which is in contrast to most DKE solvers where momentum conservation is completed with momentum correction techniques.

As an application of the NEO-2 code involving the collision matrix elements the neoclassical electron transport matrix (assuming stationary ions) for the standard tokamak with circular cross section has been evaluated. The results have shown good agreement with results of analytical theory. Moreover, effects of simplifications of the linearized collision model (e.g., reduction to a Lorentz model) have been studied in order to provide a comparison with various momentum correction techniques used for the computation of transport coefficients in stellarators. Furthermore, the NEO-2 code has been applied to compute the generalized Spitzer function in the standard tokamak taking into account finite plasma collisionality. The result has been compared to the collisionless approximation computed by the SYNCH code. This function is one of the main elements in computations of electron cyclotron current drive (ECCD) efficiency and total ECCD current. The resulting generalized Spitzer function has specific features which are pertinent to the finite plasma collisionality. They are absent in asymptotic (collisionless or highly collisional) regimes or in results drawn from interpolation between asymptotic limits. These features have the potential to improve the overall ECCD efficiency if one optimizes the microwave beam launch scenarios accordingly.

The code NEO-2 turns out to be a valuable DKE solver for ECCD problems because of the unique feature that the full linearized collision operator can be used locally. Thus the full 3D (4D) problem of local current drive efficiency can be tackled in tokamaks (stellarators). At the moment however, usage is only possible for tokamak problems due to limited speed of the code. A substantial speed-up of the code is possible with improvements of the ODE-solver and code parallelization. Such improvements are in development.

Kurzfassung

In toroidalen magnetischen Einschlusssystemen spielt der neoklassische Transport eine maßgebliche Rolle. Die vorliegende Arbeit präsentiert eine ausführliche Berechnung von Momenten des linearisierten Coulomb Stoßoperators (Stoß-Matrixelemente) mittels, zu verallgemeinerten Laguerre-Polynomen proportionalen, Testfunktionen. Diese Matrixelemente wurden in den DKE (drift kinetic equation) Solver NEO-2, der auf Integration entlang der Feldlinie beruht, direkt auf Ebene der DKE implementiert. Daher ist NEO-2 auch in der Lage, eine vollständige lokale Lösung (inklusive Diffusion der Energie und Impulserhaltung) entlang der Magnetfeldlinie zu finden. Diese Fähigkeit unterscheidet NEO-2 erheblich von den meisten DKE-Solvern, die die Impulserhaltung mittels Korrekturmethoden erst im Nachhinein sicherstellen. Als Anwendung der Matrixelemente wurde mit NEO-2 der Elektronenanteil der neoklassischen Transportmatrix (unter der Annahme stationärer Ionen) für einen Standardtokamak mit kreisförmigem Querschnitt berechnet. Die Ergebnisse zeigen eine gute Übereinstimmung mit den entsprechenden Ergebnissen der analytischen Theorie. Überdies wurde die Auswirkung vereinfachter Stoßoperatoren (z.B. Lorentzoperator) auf die Transportkoeffizienten untersucht. Dies ermöglicht für Stellaratoren hinsichtlich Impulserhaltung den Vergleich mit diversen Korrekturmethoden. Außerdem wurde mittels NEO-2 die verallgemeinerte Spitzerfunktion für einen Standardtokamak unter Berücksichtigung eines endlichen Stoßparameters (collisionality) des Plasmas berechnet und mit der stoßfreien Näherung des Codes SYNCH verglichen. Sie ist besonders wichtig bei der Berechnung der Effizienz der Stromgenerierung mittels Elektronen (electron cyclotron current drive, ECCD) und des via ECCD erzeugten Stroms. Die mit NEO-2 berechnete Spitzerfunktion weist Besonderheiten auf, die auf die endliche collisionality des Plasmas zurückzuführen sind und in asymptotischen Regimen (stoßfrei bzw. hochgradig stoßbe- stimmt), sowie in der durch Interpolation zwischen diesen Limits gewonnenen Lösung, nicht auftreten. Dieses Charakteristikum könnte dazu beitragen den Gesamtwirkungsgrad der ECCD zu verbessern, falls man den Einstrahlwinkel der Mikrowellen dementsprechend optimiert.

Für ECCD Probleme erweist sich NEO-2 als sehr nützlich, da er in der einzigartigen Lage ist, den linearisierten Stoßoperator lokal zu verwenden. Dadurch ist es überhaupt erst möglich das 3D (4D) Problem der Bestimmung der lokalen Stromtriebeffizienz in Tokamaks (Stellaratoren) zu bewältigen. Die Verwendung von NEO-2 beschränkt sich im Moment aufgrund langer Rechenzeiten auf Tokamaks. Eine Verbesserung des ODE-Solvers, sowie eine Parallelisierung des Codes sollte zu einer beträchtlichen Beschleunigung von NEO-2 führen. Diese Verbesserungen sind gerade in Entwicklung.

Dedicated to my parents

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"Das ewig Unbegreifliche an der Natur ist ihre Begreiflichkeit" 1 Albert Einstein in $Physik\ und\ Realit\"at\ [1]$

¹ "The eternal mystery of the world is its comprehensibility"

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Chapter 1

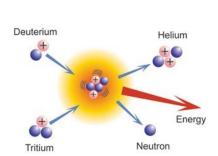
Prologue

Modern civilization is dependent on (cheap and reliable) energy and the global demand for energy is continually rising. These days roughly 85% of the worldwide energy consumption is supplied by fossil fuels [2] leading to negative effects on the environment (pollution, releasing of greenhouse gases, global warming). Beyond that, there is hardly doubt that the world is running out of fossil fuels. Therefore, in order to ensure energy supply for future generations, there is a great need to find cleaner and more sustainable energy sources that will replace coal, natural gas and oil.

In addition to nuclear fission and renewable energy means, such as solar, wind and hydro-power, nuclear fusion could also make an important contribution to the future world energy mix [2]. In particular nuclear fusion has the potential to provide (base-load) power supply offering key advantages [2–4] of, e.g., practically inexhaustible fuel (the major fuels deuterium and lithium are abundant and available around the world), no CO₂ greenhouse gas emissions (that is, no contribution to global warming) and, furthermore, future fusion power stations would be inherently safe (no meltdown possible).

The goal of controlled thermonuclear fusion is to harness on earth the process powering all stars (including our sun). The nuclear fusion in the stars is based on the proton-proton interaction, that is, hydrogen nuclei collide and fuse (through a sequence of reactions, i.e. proton-proton as well as carbon cycle [5]) into heavier helium nuclei (alpha particles) [6] releasing enormous amounts of energy in the process¹. Due to the fact that the cross section for this reaction is by far too small it cannot be exploited in a fusion reactor here on earth.

¹The sum of the rest masses of fusion products is lesser than the sum of the reactants before the reaction (mass defect). Therefore, if two light nuclei fuse to form a heavier nucleus, energy is liberated (cf. Fig. 1.1) according to Einstein's relation $\Delta E = \Delta mc^2$.



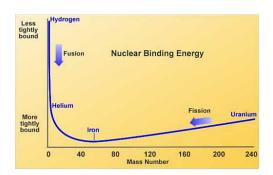


Figure 1.1: Deuterium-tritium fusion reaction (left). Energy gain from nuclear reactions (right).²

Because of its advantageous cross section the fusion reaction of primary interest for controlled thermonuclear fusion is those involving deuterium (D) and tritium (T) [7],

$$^{2}D + {^{3}T} \rightarrow {^{4}He} (3.52 \text{ MeV}) + {^{1}n} (14.06 \text{ MeV}),$$

taking place at lowest plasma temperatures ($\approx 10 \text{ keV}$) compared to other fusion reactions (see Figure 1.1). Since tritium is radioactive (with the half-life of 12.3 years) it does not occur naturally and, therefore, must be bred by lithium in the blanket surrounding the plasma using reactions such as [5]

$$^{6}\text{Li} + ^{1}\text{n} \rightarrow ^{4}\text{He} + ^{3}\text{T} + 4.80 \text{ MeV}$$

 $^{7}\text{Li} + ^{1}\text{n} \rightarrow ^{4}\text{He} + ^{3}\text{T} + ^{1}\text{n} - 2.47 \text{ MeV}.$

The following reactions might be preferred from an economic and environmental point of view (e.g. no tritium necessary), however, they possess less favorable reaction rates, require considerably higher temperatures and provide at the same pressure only 1 % of the D-T fusion power density [5],

$$^{2}D + ^{2}D \rightarrow ^{3}He (0.82 \text{ MeV}) + ^{1}n (2.45 \text{ MeV}) 50\% \text{ probability}$$
 $^{2}D + ^{2}D \rightarrow ^{3}T (1.01 \text{ MeV}) + ^{1}H (3.03 \text{ MeV}) 50\% \text{ probability}$ $^{2}D + ^{3}He \rightarrow ^{4}He (3.67 \text{ MeV}) + ^{1}H (14.67 \text{ MeV}).$

A D-T plasma has to meet the following requirements in order to yield net fusion energy from a reactor - the product of density n_i and energy confinement time τ_E of the fuel ions has to be $n_i \tau_E \ge 1.5 \times 10^{20} \text{sm}^{-3}$ (Lawson criterion)

²Source left image: http://www.iter.org/sci/whatisfusion Source right image: http://www.jet.efda.org/faq/fusion-principles

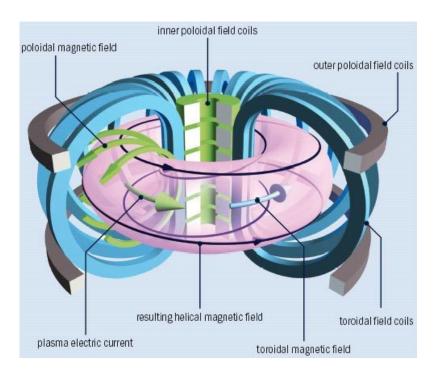


Figure 1.2: Scheme of the tokamak principle³

as well as the critical ion temperature T_i is approximately 10 kev (over 100 million degrees) [8].

In principle two different paths are being investigated in order to achieve controlled thermonuclear fusion on earth, namely, inertial confinement and, perhaps more promising, magnetic confinement. In inertial confinement fusion small and frozen pellets of D-T are compressed to very high densities and heated to fusion conditions by means of intense lasers or high power particle beams (so-called energy drivers). The heating pulses are typically 1 to 10 ns long [9].

A concept fundamentally different from that is the magnetic confinement fusion, where a low density plasma (fully ionized gas) is confined in a strong magnetic field relying on the fact that the magnetic field can influence the motion of the charged particles and isolate them from the inner wall of the containment vessel. The most advanced magnetic confinement systems are toroidal, namely the tokamak [10,11] and the stellarator [12].

In a tokamak (a schematic diagram is shown in Figure 1.2) a toroidal magnetic field is produced by currents in external field coils surrounding the vacuum

 $^{^3} Source: http://ec.europa.eu/research/energy/euratom/publications/fusion/index_en.htm/$

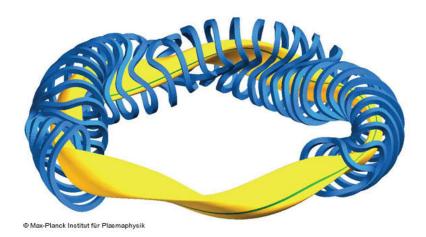


Figure 1.3: Plasma and (non-planar and non-circular) magnetic coils of the advanced modular stellarator $W7-X^4$

vessel and a poloidal magnetic field is generated by a current flowing through the plasma. The combined total magnetic field lines are helically twisted around the torus center. Since the toroidal current is induced by transformer action (the plasma itself acts as the secondary winding) a tokamak is intrinsically a pulsed device. Moreover, the large plasma current can drive large scale plasma instabilities, the so-called disruptions (an abrupt termination of the discharge where magnetic confinement is destroyed [13]).

Currently, the largest tokamak experiments are the JET (Joint European Torus) [14], based in Culham (Great Britain) and the JT-60U [15, 16] built in Naka (Japan).

In a stellarator the helical twist of the confining magnetic field is generated exclusively by currents flowing in external field coils. Consequently, stellarators are non toroidally symmetric (i.e., fully three dimensional) plasma confinement devices⁵. Due to the absence of a net toroidal current, stellarators have the potential to be operated in steady-state and are believed to be disruption-free [17]. At present, the largest stellarator is the LHD (Large Helical Device) [18] in Toki, Gifu (Japan). A schematic diagram of the advanced stellarator W7-X (Wendelstein 7-X) [19, 20], that is currently being built in Greifswald (Germany), is shown in Figure 1.3.

The next major step in fusion research is the ITER tokamak [5] (International Thermonuclear Experimental Reactor) which is currently being built in

⁴Source: http://www.ipp.mpg.de/ippcms/eng/pr/forschung/w7x/index.html

 $^{^5\}mathrm{A}$ great advantage of the dough nut-shaped tokamak is the axisymmetry of the configuration.

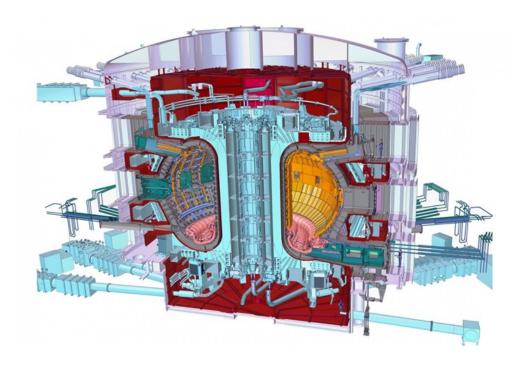


Figure 1.4: A cutaway view of the future ITER Tokamak⁶. © ITER Organization

Cadarache (France) with the aim to prove the scientific and technological feasibility producing commercial energy from nuclear fusion [21] (see Figure 1.4). ITER is projected to generate 500MW fusion power, ten times more than it consumes as well as to test key technologies required for a future fusion power plant [5,21] (the so-called DEMO, an industrial demonstration reactor).

In toroidal magnetic confinement devices substantial external⁷ heating systems are required in order to bring the plasma to ignition temperatures, that is, to temperatures where self-heating due to α -particles maintains the thermonuclear fusion. The following two main techniques have therefore been developed: Neutral-beam injection (or NBI) as well as radio-frequency (RF) heating. In NBI, high-energy neutral atoms (typically hydrogen isotopes) are injected across the confining magnetic field into the plasma transferring their energy in repeated collisions to the plasma ions and electrons. In RF heating, energy is transferred to the charged plasma particles via resonant

⁶Source: http://fusionforenergy.europa.eu/mediacorner/imagegallery.aspx?id=25

⁷In tokamaks the heat produced by the induced toroidal plasma current (ohmic heating) is insufficient to reach self-sustained fusion and in stellarators, actually, all the energy needed to attain the temperatures required for fusion has to be provided by external heating.

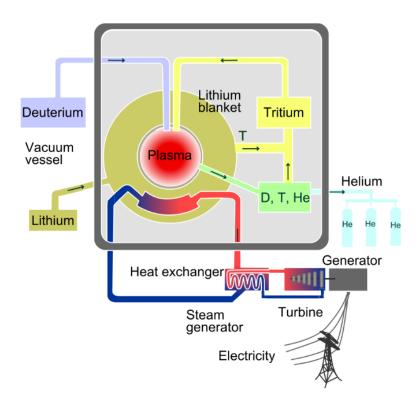


Figure 1.5: Conceptual layout of a fusion power plant⁸

absorption of high-power electromagnetic waves at appropriate frequencies (viz. the cyclotron frequencies of ions and electrons) [5,7,13].

Finally, Figure 1.5 shows the principle scheme of a magnetic fusion power plant based on the D-T reaction. The hot plasma is surrounded by the first wall, followed by the so-called blanket and the vacuum vessel protecting the superconducting magnetic coils from the heat and high-energy neutron fluxes produced by fusion reactions. Since the neutrons are not confined by the magnetic field they escape the plasma, pass the first wall and penetrate the lithium blanket where they are slowed down converting their kinetic energy to heat. The heat in turn is removed by means of a coolant (helium or liquid metals) and is used to generate electricity. Moreover, the neutrons which enter the blanket are absorbed by lithium in order to breed tritium which is then used as fuel [5, 13, 21].

A drawback in using the D-T fusion reaction is the induced radioactivity of the reactor materials (particularly the blanket and vessel structure) caused by the

⁸Source: http://www.efda.org/multimedia/animations.htm

fast neutrons. However, the application of advanced, so-called low-activation, structural materials (which are currently under development) will largely reduce the total radioactivity. It is expected that most reactor materials can be recycled after a decay time of about a hundred years after the end of the power plant's life [2,5,13]. Another problem in a D-T reactor is the radioactive tritium which is difficult to contain and which requires careful handling. The total amount of tritium present in the plant is estimated to be on the order of a few kilograms (only a few grams in the plasma) and is generated in a closed fuel cycle. Nonetheless, future nuclear fusion power plants must preclude accident-caused release of tritium inventory [2,5,21].

Chapter 2

Introduction

In toroidal magnetic confinement systems, such as tokamaks and stellarators, transport of particles and energy plays a significant role. In principle, plasma transport can be divided into three different kinds of transport mechanisms, namely the classical, the neoclassical and the anomalous transport. While classical and neoclassical transport are driven by Coulomb collisions between charged particles the anomalous transport is caused by turbulent processes (e.g., fluctuating electromagnetic fields, micro-instabilities).

On the collisional transport the classical flux results from the interaction of Coulomb scattering with particle gyromotion which is perpendicular to the magnetic field (perpendicular friction) while neoclassical diffusion is determined by the interaction of Coulomb scattering with guiding-center drift motion. This motion is primarily along the magnetic field, thus neoclassical transport is associated with parallel friction [22, 23].

This work concentrates on the investigation of neoclassical transport processes in tokamaks and stellarators, more precisely, on the evaluation of the neoclassical transport matrix and the generalized Spitzer function.

Accurate computations of axisymmetric and non-axisymmetric neoclassical transport coefficients, bootstrap current and the generalized Spitzer function is an important problem for stellarator optimization, generation of neoclassical data bases, and modeling of current drive. Based on the field line integration technique [24], the generalized drift kinetic equation solver NEO-2 has been developed for this purpose [25, 26]. This code solves the linearized drift kinetic equation in regimes where the effect of electric field on transport and bootstrap coefficients is negligible.

Recently this code has been upgraded for computations of the full transport matrix, that is, NEO-2 has been generalized for a full linearized collision operator describing all aspects of Coulomb collisions including energy scattering and momentum conservation. Applying the full linearized collision operator

represents a considerable improvement to the previous version of the code, where only the Lorentz (pitch-angle scattering) operator was implemented and, furthermore, is a prerequisite for a complete description of neoclassical transport and linear current drive efficiency (e.g., for solving the generalized Spitzer-Härm problem in arbitrary stellarator geometry). The generalized Spitzer-Härm function serves as current drive efficiency for ECCD and other methods with a small distortion of the distribution function. Currently, two limiting cases of this function are mainly used in ECCD modeling: (i) high-collisionality limit (homogeneous magnetic field limit) and (ii) low collisionality limit (bounce averaged Spitzer-Härm function). The intermediate cases are obtained by some heuristic matching formulas. Detailed knowledge about the collisionality dependence of this function is important for interpretation of present-day experiments and also for reactor modeling in the case of ECCD with near perpendicular microwave beam injection.

The implementation of the full linearized collision operator in NEO-2 is in contrast to most DKE solvers where momentum conservation is completed with so-called momentum correction techniques (based on three monoenergetic transport coefficients) applied to flux surface averaged quantities [27,28]. Thus, local information within a flux surface is lost. This makes NEO-2 especially suited for ECCD computations where power deposition is highly localized.

The motivation for the work presented in this thesis was to provide the moments of the full linearized Coulomb collision operator (also called collision matrix elements) which are used in the code NEO-2 to solve the linearized drift kinetic equation. In the following an elaborated derivation of these matrix elements is shown.

Finally, it has to be pointed out that the development of the solver itself was not part of this work.

The thesis is organized as follows.

In Chapter 3 the neoclassical electron transport matrix relating the neoclassical fluxes and the thermodynamical forces is derived. The corresponding transport coefficients are represented in thermal as well as in monoenergetic form and it is shown that for the Lorentz operator the thermal transport coefficients can be obtained from the monoenergetic ones using a convolution over energy. Furthermore, it is demonstrated that the transport matrix is Onsager symmetric and that it depends on the choice of fluxes and forces. In Chapter 4 a brief description of the adjoint approach for ECCD computations is given and it is shown how the generalized Spitzer function is calculated in the NEO-2 code.

The main part of this work is presented in Chapter 5, namely the calculation of the collision matrix elements using the full linearized Coulomb collision operator. The test particle matrix elements are computed in terms of the orthonormal test functions φ_m proportional to the associated Laguerre polynomials whereas the field particle matrix elements are evaluated in the Burnett function basis first followed by a transformation to the φ_m -basis. Additionally, the asymptotic behavior of the matrix elements is studied for the case when the ratio of particle masses $m_a/m_b \ll 1$. Moreover, recurrence relations are provided allowing for fast numerical evaluation of the collision matrix elements and their numerical implementation is briefly described.

In Chapter 6 a standard problem in plasma physics, namely the calculation of the classical Spitzer conductivity, is solved which serves as a test case for the accuracy of the matrix elements.

Chapter 7 compares the results obtained from analytical formulas representing the neoclassical transport matrix in the low-collisionality limit in an axisymmetric test configuration with the corresponding numerical findings evaluated by means of the NEO-2 code.

In Chapter 8 the computational results of the neoclassical transport matrix and generalized Spitzer function in a standard tokamak with finite collisionality obtained with the NEO-2 code are presented and discussed. Besides, a brief description of the code NEO-2 is given.

Chapter 9, finally, contains the conclusions of this thesis.

In the appendices two complete sets of orthonormal functions applied in this work are introduced (the test functions φ_m as well as the Burnett functions). In addition, various representations and properties of the Coulomb collision operator are briefly reviewed. As an important by-product of this work the Trubnikov potentials as well as the Braginskii matrix elements are calculated in the Burnett function basis and presented in a compact form. Finally, in the last part of the appendix the construction of a test configuration with circular cross section (standard tokamak) is shown which is used for comparison between numerical results obtained by the NEO-2 code and the analytical predictions in the axisymmetric limit.

2.1 Publications associated with this thesis

In the following the list of articles as well as contributions to European Physical Society conferences and International Stellarator Workshops co-authored by the author of this thesis are presented.

2.1.1 Peer reviewed journal articles

- Recent progress in NEO-2 A code for neoclassical transport computations based on field line tracing
 - W. Kernbichler, S. V. Kasilov, G. O. Leitold, V. V. Nemov and K. Allmaier, Plasma and Fusion Research 3, S1061 (2008)
- Generalized Spitzer Function with Finite Collisionality in Toroidal Plasmas
 - W. Kernbichler, S. V. Kasilov, G. O. Leitold, V. V. Nemov and N. B. Marushchenko, Contrib. Plasma Phys. **50**, 761 (2010)

2.1.2 Conference proceedings

- Calculation of neoclassical transport in stellarators with finite collisionality using integration along magnetic field lines
 W. Kernbichler, S. V. Kasilov, G. O. Leitold and V. V. Nemov, 32nd EPS Conference on Plasma Phys. and Contr. Fusion, Tarragona, 27 June–1 July 2005, ECA 29C, P-1.111 (2005)
- Computation of neoclassical transport in stellarators with finite collisionality
 W. Kernbichler, S. V. Kasilov, G. O. Leitold, V. V. Nemov and K. Allmaier, 15th International Stellarator Workshop, Madrid, 3–7 October, 2005, P2-15 (2005)
- Computation of neoclassical transport in stellarators using the full linearized Coulomb collision operator
 W. Kernbichler, S. V. Kasilov, G. O. Leitold, V. V. Nemov and K. Allmaier, 33rd EPS Conference on Plasma Physics, Rome, 19–23 June 2006, ECA 30I, P-2.189 (2006)
- ICNTS Benchmarking of Momentum Correction Techniques
 C. D. Beidler, M. Yu. Isaev, S. V. Kasilov, W. Kernbichler, G. O. Leitold,
 H. Maaßberg, S. Murakami, V. V. Nemov, D. A. Spong and V. Tribaldos,
 16th International Stellarator/Heliotron Workshop 2007, Ceratopia Toki,
 Japan, 15–19 October 2007, P2-030 (2007)
- Recent progress in NEO-2 A code for neoclassical transport computations based on field line tracing
 W. Kernbichler, S. V. Kasilov, G. O. Leitold, V. V. Nemov and K. Allmaier, 16th International Stellarator/Heliotron Workshop 2007, Ceratopia Toki, Japan, 15–19 October 2007, P2-022 (2007)

Current Drive Calculations: Benchmarking Momentum Correction and Field-Line Integration Techniques
M. Romé, C. D. Beidler, S. V. Kasilov, W. Kernbichler, G. O. Leitold, H. Maaßberg, N. B. Marushchenko, V. V. Nemov and Yu. Turkin, 35th EPS Conference on Plasma Physics, Sofia, June 29–July 3 2009, ECA 33E, P-1.136 (2009)

2.2 Publications related to neoclassical transport

In addition to the above mentioned publications, the author of the present thesis contributed to the following papers and conference proceedings on neoclassical transport (though not directly related to the thesis):

2.2.1 Peer reviewed journal articles

- The ∇B drift velocity of trapped particles in stellarators
 V. V. Nemov, S. V. Kasilov, W. Kernbichler and G. O. Leitold, Phys. Plasmas 12, 112507 (2005)
- Variance reduction in computations of neoclassical transport in stellarators using a δf method
 K. Allmaier, S. V. Kasilov, W. Kernbichler and G. O. Leitold, Phys. Plasmas 15, 072512 (2008)
- Poloidal motion of trapped particle orbits in real-space coordinates
 V. V. Nemov, S. V. Kasilov, W. Kernbichler and G. O. Leitold, Phys. Plasmas 15, 052501 (2008)
- Benchmarking Results From the International Collaboration on Neoclassical Transport in Stellarators ICNTS
 C. D. Beidler, K. Allmaier, M. Yu. Isaev, S. V. Kasilov, W. Kernbichler, G. O. Leitold, H. Maaßberg, D. R. Mikkelsen, S. Murakami, M. Schmidt,

D. A. Spong, V. Tribaldos, A. Wakasa, submitted to Nucl. Fusion (2010)

2.2.2 Conference proceedings

Consistent Recalculation of MHD Equilibria from VMEC, B. Seiwald, G. O. Leitold, W. Kernbichler and S. V. Kasilov, 28th EPS Conference on Contr. Fusion and Plasma Phys., Funchal, 18–22 June 2001, ECA 25A, 769 (2001)

- Self Consistent Recalculation of MHD Equilibria from VMEC, B. Seiwald, G. O. Leitold, W. Kernbichler and S. V. Kasilov, 13th International Stellarator Workshop, Canberra, Feb 25– Mar 1, 2002, Paper No. PIIA.18 (2002)
- Neoclassical Transport Calculations for Optimization Studies
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 17–21 June 2002, ECA 26B, P-2.100 (2002)
- Evaluation of the Bootstrap Current in Stellarators
 W. Kernbichler, S. V. Kasilov, V. V. Nemov, G. Leitold and M. F. Heyn,
 PLASMA PHYSICS: 11th International Congress on Plasma Physics:
 ICPP2002, Sydney (Australia), 15-19 July 2002, AIP Conference Proceedings Subseries: Plasma Physics 669, 492-495 (2003)
- Simple criteria for optimization of trapped particle confinement in stellarators
 V. V. Nemov, S. V. Kasilov, W. Kernbichler and G. O. Leitold, 32nd EPS Conference on Plasma Phys. and Contr. Fusion, Tarragona, 27 June–1 July 2005, ECA 29C, P-1.109 (2005)
- Additional criteria for optimization of trapped particle confinement in stellarators
 V. V. Nemov, S. V. Kasilov, W. Kernbichler and G. O. Leitold, 15th International Stellarator Workshop, Madrid, 3–7 October 2005, P2-14 (2005)
- Assessment of the trapped particle confinement in optimized stellarators
 V. V. Nemov, W. Kernbichler, S. V. Kasilov, G. O. Leitold and L. P. Ku,
 33rd EPS Conference on Plasma Physics, Rome, 19–23 June 2006, ECA
 30I, P-4.164 (2006)
- Computations of neoclassical transport in stellarators using a δf method with reduced variance
 K. Allmaier, S. V. Kasilov, W. Kernbichler, G. O. Leitold and V. V. Nemov, 16th International Stellarator/Heliotron Workshop 2007, Toki, Japan, 15–19 October 2007, P2-021 (2007)

2.2. PUBLICATIONS RELATED TO NEOCLASSICAL TRANSPORT 15

- Variance reduction in computations of neoclassical transport in stellarators using a δf method
 K. Allmaier, S. V. Kasilov, W. Kernbichler, G. O. Leitold and V. V. Nemov, 34th EPS Conference on Plasma Physics, Warsaw, Poland, July 2–6 2007, ECA 31F, P-4.041 (2007)
- δf Monte Carlo computations of neoclassical transport in stellarators with reduced variance
 K. Allmaier, S. V. Kasilov, W. Kernbichler and G. O. Leitold, 35th EPS Conference on Plasma Phys. Hersonissos, 9 - 13 June 2008, ECA 32D, P-4.017 (2008)
- Poloidal drift of trapped particle orbits in real-space coordinates
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 32D, P-5.021 (2008)

Chapter 3

Neoclassical transport matrix

In the following chapter a formalism is developed, based on the linearized drift kinetic equation, which allows for a compact representation of the neoclassical transport matrix relating the neoclassical fluxes to the thermodynamical forces which drive them. The corresponding matrix elements are presented in thermal as well as in monoenergetic form. Furthermore, a proof of Onsager symmetry of the transport matrix is given and it is shown how the transport matrix has to be transformed for two different sets of thermodynamical forces.

3.1 Drift kinetic equation

The first-order gyrophase-averaged distribution function (defined as the small deviation from lowest-order Maxwellian) for particles of species a, f_{a1} , is determined by the linearized drift kinetic equation (see, e.g., Reference 22)

$$v\lambda \frac{\partial f_{a1}}{\partial s} + V^{\psi} \frac{\partial f_{a0}}{\partial \psi} - \frac{e_a v\lambda E_{\parallel}^{(A)}}{T_a} f_{a0} = \mathcal{C}_a^l[f_{a1}], \tag{3.1}$$

where the linearized Coulomb collision operator \mathcal{C}_a^l is defined by

$$C_a^l[f_{a1}] = \sum_b \left(C_{ab}[f_{a1}, f_{b0}] + C_{ab}[f_{a0}, f_{b1}] \right) , \qquad (3.2)$$

neglecting terms quadratic in f_{a1} and f_{b1} . Here, f_{a0} and f_{b0} represent Maxwellian distribution functions satisfying $C_{ab}[f_{a0}, f_{b0}] = 0$ for equal species temperatures $T_a = T_b$. The first and the last term on the RHS of Eq. (3.2) correspond to the differential and integral part of the collision operator, respectively. In Eq. (3.1), ψ is a flux surface label, s is the distance counted along the magnetic field line, $\lambda = v_{\parallel}/v$ is the pitch angle variable, e_a is the

charge, $E_{\parallel}^{(A)}$ is the induced parallel electric field and $V^{\psi} = \mathbf{V} \cdot \nabla \psi$ is the radial component of the drift velocity [24]

$$V^{\psi} = -\frac{v^2}{\omega_{c0}} \lambda \frac{\partial}{\partial \eta} \left(\frac{\lambda}{\hat{B}} \hat{V}_G \right) , \qquad (3.3)$$

where $\eta = (1 - \lambda^2)/\hat{B}$, $\hat{B} = B/B_0$ is the magnetic field module normalized to a reference magnetic field B_0 , $\omega_{c0} = eB_0/(m_e c)$ and

$$\hat{V}_G = \frac{1}{3} \left(\frac{4}{\hat{B}} - \eta \right) |\nabla \psi| k_g , \qquad (3.4)$$

with k_G being the geodesic curvature.

The local Maxwellian distribution function is represented by

$$f_{e0}(\psi, x) = \frac{n_e}{\pi^{3/2} v_{te}^3} e^{-x^2}, \tag{3.5}$$

where n_e is the density, $v_{te} = \sqrt{2T_e/m_e}$ is the thermal speed and $x = v/v_{te}$ is the normalized particle speed, respectively. Here it has to be noted that the temperature, the density and the electrostatic potential Φ are assumed to be constant on magnetic flux surfaces. From Eq. (3.5) one obtains for the radial derivative (at constant total energy $E = mv^2/2 + e_a\Phi$) of the Maxwellian,

$$\frac{\partial f_{e0}(\psi, x)}{\partial \psi} = A_1(\psi) f_{e0}(\psi, x) + A_2(\psi) x^2 f_{e0}(\psi, x), \tag{3.6}$$

with A_1 and A_2 being the thermodynamic forces

$$A_1(\psi) = \frac{1}{n_e} \frac{\partial n_e}{\partial \psi} - \frac{3}{2T_e} \frac{\partial T_e}{\partial \psi} - \frac{e}{T_e} \frac{\partial \Phi}{\partial \psi}$$
 (3.7)

$$A_2(\psi) = \frac{1}{T_e} \frac{\partial T_e}{\partial \psi} \,. \tag{3.8}$$

Using the fact that in neoclassical theory the induced parallel electric field $E_{\parallel}^{(A)}$ is often replaced by $B\langle E_{\parallel}^{(A)}B\rangle/\langle B^2\rangle$ [22] the electron component of Eq. (3.1) can be rewritten as

$$v\lambda \frac{\partial f_{e1}}{\partial s} - \mathcal{C}_e^l[f_{e1}]$$

$$= -f_{e0} \left[V^{\psi} A_1(\psi) + V^{\psi} x^2 A_2(\psi) + v\lambda \hat{B} \frac{e}{T_e} \frac{\langle E_{\parallel}^{(A)} \hat{B} \rangle}{\langle \hat{B}^2 \rangle} \right]$$

$$= -f_{e0} \left[\frac{V^{\psi}}{\langle |\nabla \psi| \rangle} A_1(r) + \frac{V^{\psi}}{\langle |\nabla \psi| \rangle} x^2 A_2(r) - v\lambda \hat{B} A_3(r) \right].$$
 (3.10)

In Eq. (3.10) the thermodynamic forces A_1 and A_2 have been expressed as functions of the effective radius r by means of the definition $\partial/\partial\psi$ $\langle |\nabla \psi| \rangle^{-1} \partial / \partial r$, and the driving force

$$A_3 = -\frac{e}{T_e} \frac{\langle E_{\parallel}^{(A)} \hat{B} \rangle}{\langle \hat{B}^2 \rangle} \tag{3.11}$$

has been introduced. Here, the notation $\langle \cdot \rangle$ denotes the flux surface average which can be evaluated using (see, e.g., [24])

$$\frac{\langle G \rangle}{\langle H \rangle} = \lim_{L \to \infty} \int_0^L \frac{\mathrm{d}s}{\hat{B}} G \left(\int_0^L \frac{\mathrm{d}s}{\hat{B}} H \right)^{-1}. \tag{3.12}$$

Upon defining the quantities Q_i^{σ} ,

$$Q_1^{\sigma} = -\frac{V^{\psi}}{\langle |\nabla \psi| \rangle} \tag{3.13}$$

$$Q_2^{\sigma} = x^2 Q_1^{\sigma}$$

$$Q_3^{\sigma} = \sigma v |\lambda| \hat{B},$$

$$(3.14)$$

$$Q_3^{\sigma} = \sigma v |\lambda| \hat{B}, \tag{3.15}$$

with σ being the sign of v_{\parallel} , the drift kinetic equation becomes

$$\sigma v |\lambda| \frac{\partial f_{e1}^{\sigma}}{\partial s} - \mathcal{C}_{e}^{l}[f_{e1}^{\sigma}] = f_{e0} \left[Q_{1}^{\sigma} A_{1}(r) + Q_{2}^{\sigma} A_{2}(r) + Q_{3}^{\sigma} A_{3}(r) \right]. \tag{3.16}$$

Equations (3.13)-(3.15) may also be written via the compact notation

$$Q_j^{\sigma} = v_{te} \beta_j x^{2j - 5\delta_{3j}} |\lambda| q_j^{\sigma}, \quad j = 1, 2, 3$$
 (3.17)

with

$$\beta_1 = \beta_2 = \frac{\rho_{e0}}{\langle |\nabla \psi| \rangle} , \qquad \beta_3 = 1 ,$$
 (3.18)

 $\rho_{e0} = v_{te}/\omega_{c0}$ is the electron Larmor radius, and where the abbreviations

$$q_1^{\sigma} = q_2^{\sigma} \equiv \frac{\partial}{\partial \eta} \left(\frac{|\lambda|}{\hat{B}} \hat{V}_G \right)$$
 (3.19)

$$q_3^{\sigma} \equiv \sigma \hat{B} \tag{3.20}$$

have been introduced.

Because Eq. (3.16) for f_{e1}^{σ} is linear, the solution is linear in the driving forces and can be formally presented as a superposition of A_j ,

$$f_{e1}^{\sigma} = f_1^{\sigma} A_1 + f_2^{\sigma} A_2 + f_3^{\sigma} A_3 , \qquad (3.21)$$

where the functions f_i^{σ} are defined as the solutions of the single-drive problems

$$\sigma v |\lambda| \frac{\partial f_j^{\sigma}}{\partial s} - \mathcal{C}_e^l[f_j^{\sigma}] = f_{e0}Q_j^{\sigma}, \quad \text{for} \quad j = 1, 2, 3.$$
 (3.22)

Here it is convenient to introduce the normalized functions \hat{f}_i^{σ} via

$$f_j^{\sigma} = \beta_j \hat{f}_j^{\sigma}. \tag{3.23}$$

The energy dependence of the perturbation of the normalized distribution function is now approximated by an expansion over a finite number of orthonormal test functions φ_m (see Appendix A), that is

$$\hat{f}_{j}^{\sigma}(\psi, s, x, \lambda) \approx f_{e0}(\psi, x) \sum_{m=0}^{M} f_{m}^{\sigma,(j)}(\psi, s, \lambda) \varphi_{m}(x). \tag{3.24}$$

These functions are defined as follows,

$$\varphi_m(x) \equiv \pi^{3/4} \sqrt{\frac{2\Gamma(m+1)}{\Gamma(m+5/2)}} L_m^{(3/2)}(x^2) ,$$
(3.25)

where $L_m^{(3/2)}$ represents the associated Laguerre polynomials [29] of the order 3/2. Upon multiplication of Eq. (3.22) on the left by the basis function φ_m followed by an integration over $\int_0^\infty \mathrm{d}v v^3$ the linearized drift kinetic equation for the single-drive problems is transformed to a set of coupled two dimensional ordinary differential equations for the coefficients $f_m^{\sigma,(j)}$ (see Chapter 5),

$$\sigma \frac{\partial f_{m}^{\sigma,(j)}}{\partial s} - \kappa \sum_{m'=0}^{M} \left\{ \nu_{mm'}^{e} \hat{\mathcal{L}} f_{m'}^{\sigma,(j)} + \hat{\mathcal{K}}_{mm'}^{e} f_{m'}^{\sigma,(j)} + \frac{1}{|\lambda|} D_{mm'}^{e} f_{m'}^{\sigma,(j)} \right\} = a_{m}^{(j)} q_{j}^{\sigma} , \quad (3.26)$$

with the pitch-angle scattering operator

$$\hat{\mathcal{L}}f_{m'}^{\sigma,(j)} = \frac{1}{2|\lambda|} \frac{\partial}{\partial \lambda} (1 - \lambda^2) \frac{\partial}{\partial \lambda} f_{m'}^{\sigma,(j)}(\psi, s, \lambda)
= 2 \frac{\partial}{\partial \eta} \left(\frac{\eta|\lambda|}{\hat{B}} \right) \frac{\partial}{\partial \eta} f_{m'}^{\sigma,(j)}(\psi, s, \eta) ,$$
(3.27)

and the integral part of the linearized collision operator

$$\hat{\mathcal{K}}_{mm'}^{e} f_{m'}^{\sigma,(j)} = \frac{1}{|\lambda|} \sum_{\ell=0}^{L} I_{mm'}^{(\ell)} P_{\ell}(\lambda) \int_{-1}^{1} d\lambda' P_{\ell}(\lambda') f_{m'}^{\sigma',(j)}(\psi, s, \lambda') . \tag{3.28}$$

Here, P_{ℓ} are Legendre polynomials, $\kappa \equiv 1/(v_{te}\tau_{ee})$ is the collisionality parameter (with $v_{te}\tau_{ee} \equiv l_c$ being the electron mean free path due to electron electron collisions alone [30]) and τ_{ee} is the collision time

$$\tau_{ee} = \frac{3m_e^2 v_{te}^3}{16\sqrt{\pi}n_e e^4 \ln \Lambda},\tag{3.29}$$

where $\ln \Lambda$ denotes the Coulomb logarithm. The quantities $\nu_{mm'}^e$, $I_{mm'}^{(\ell)}$, $D_{mm'}^e$ (which is calculated from the energy scattering part of $\mathcal{C}_{eb}[f_{e1}, f_{b0}]$) and $a_m^{(j)}$ are matrix elements independent of plasma parameters and their calculation is deferred to Chapter 5. In principle, the total effect on the electrons is given by a sum over all background species b (including electrons), that is

$$\nu_{mm'}^e = \sum_b \nu_{mm'}^{eb} \tag{3.30}$$

$$D_{mm'}^{e} = \sum_{b} D_{mm'}^{eb} \tag{3.31}$$

$$\hat{\mathcal{K}}^{e}_{mm'} = \sum_{b} \hat{\mathcal{K}}^{eb}_{mm'}. \tag{3.32}$$

In this work the transport coefficients are computed only for the electron component assuming the ions to be immobile, that is Eqs. (3.30)-(3.32) can be replaced by

$$\nu_{mm'}^e = \nu_{mm'}^{ee} + Z_{\text{eff}} \nu_{mm'}^{e\infty} \tag{3.33}$$

$$D_{mm'}^e = D_{mm'}^{ee} (3.34)$$

$$\nu_{mm'}^{e} = \nu_{mm'}^{ee} + Z_{\text{eff}} \nu_{mm'}^{e\infty}$$

$$D_{mm'}^{e} = D_{mm'}^{ee}$$

$$\hat{\mathcal{K}}_{mm'}^{e} = \hat{\mathcal{K}}_{mm'}^{ee} ,$$
(3.33)
$$(3.34)$$

with the effective charge

$$Z_{\text{eff}} = \frac{\sum_s Z_s^2 n_s}{\sum_s Z_s n_s},\tag{3.36}$$

and where a quasineutral plasma, $n_e = \sum_s Z_s n_s$, has been assumed.

In the code NEO-2, Eq. (3.26) is solved on a single field line using the method of Green's functions computed with the help of an adaptive third order conservative finite-difference scheme over the normalized perpendicular adiabatic invariant η . For an advanced description of this method see, e.g., References 25, 26 and 31 as well as Chapter 8.1.

3.2 Transport coefficients

The neoclassical transport fluxes of particles, energy and parallel electron current density are derived from the first order distribution function. Here, $\langle \Gamma_a \cdot \nabla r \rangle = \langle \Gamma_a^r \rangle$ and $\langle \mathbf{Q}_a \cdot \nabla r \rangle = \langle Q_a^r \rangle$ are surface averaged radial particle and energy flux densities defined as total particle and energy fluxes divided by the flux surface area and j_{\parallel} is the total parallel electron current density. Accordingly, the particle flux is expressed as

$$\langle \Gamma_e^r \rangle = \frac{\langle \int d^3 v V^{\psi} f_{e1} \rangle}{\langle |\nabla \psi| \rangle}$$

$$= -\sum_{k=1}^{3} \frac{1}{\omega_{c0} \langle |\nabla \psi| \rangle} \langle \int d^3 v v^2 |\lambda| \frac{\partial}{\partial \eta} \left(\frac{|\lambda|}{\hat{B}} \hat{V}_G \right) f_k^{\sigma} \rangle A_k$$

$$= -\sum_{k=1}^{3} \frac{v_{te} \rho_{e0}}{\langle |\nabla \psi| \rangle} \langle \int d^3 v x^2 |\lambda| q_1^{\sigma} f_k^{\sigma} \rangle A_k , \qquad (3.37)$$

the energy flux reads

$$\langle Q_e^r \rangle = \frac{\langle \int d^3 v (m v^2 / 2) V^{\psi} f_{e1} \rangle}{\langle |\nabla \psi| \rangle}$$

$$= -T_e \sum_{k=1}^3 \frac{v_{te} \rho_{e0}}{\langle |\nabla \psi| \rangle} \langle \int d^3 v x^4 |\lambda| q_2^{\sigma} f_k^{\sigma} \rangle A_k , \qquad (3.38)$$

and the surface averaged parallel current density is given by

$$\langle j_{\parallel} \hat{B} \rangle = -e \left\langle \hat{B} \int d^{3}v v_{\parallel} f_{e1} \right\rangle$$

$$= -\sum_{k=1}^{3} e \left\langle \int d^{3}v \sigma \hat{B}v |\lambda| f_{k}^{\sigma} \right\rangle A_{k}$$

$$= \sum_{k=1}^{3} e v_{te} \left\langle \int d^{3}v x |\lambda| q_{3}^{-\sigma} f_{k}^{\sigma} \right\rangle A_{k}, \qquad (3.39)$$

respectively. With the following definitions,

$$I_1 \equiv \langle \Gamma_e^r \rangle , \qquad I_2 \equiv \frac{\langle Q_e^r \rangle}{T_e} , \qquad I_3 \equiv -\frac{\langle j_{\parallel} \hat{B} \rangle}{e} , \qquad (3.40)$$

the neoclassical fluxes in Eqs. (3.37)-(3.39) may also be expressed as

$$I_j = -\left\langle \int d^3 v Q_j^{-\sigma} f_{e1} \right\rangle, \tag{3.41}$$

where Eq. (3.17) has been applied. By means of Eq. (3.21) and upon defining the electron transport coefficients L_{jk}^{e} (electron transport matrix) the relation between fluxes and thermodynamical forces can be written in the form

$$I_j = -\sum_{k=1}^3 L_{jk}^e A_k, (3.42)$$

with

$$L_{jk}^{e} \equiv \left\langle \int d^{3}v Q_{j}^{-\sigma} f_{k}^{\sigma} \right\rangle. \tag{3.43}$$

Substituting into Eq. (3.43) the volume element in velocity space,

$$\int d^3 v = \pi v_{te}^3 \hat{B} \sum_{\sigma=\pm 1} \int_0^\infty dx x^2 \int_0^{1/\hat{B}(s)} d\eta \frac{1}{|\lambda|},$$
 (3.44)

and using again the normalization $f_k^{\sigma} = \beta_k \hat{f}_k^{\sigma}$ one gets for the transport coefficients the equation

$$L_{jk}^{e} = 4\pi v_{te}^{4} \beta_{j} \beta_{k} \int_{0}^{\infty} dx x^{2(j+1)-5\delta_{3j}} \sum_{\sigma=\pm 1} \left\langle \frac{\hat{B}}{4} \int_{0}^{1/\hat{B}} d\eta q_{j}^{-\sigma} \hat{f}_{k}^{\sigma} \right\rangle , \qquad (3.45)$$

with j, k = 1, 2, 3. Formally, the transport coefficients may be obtained by evaluating these integrals once the distribution function \hat{f}_k^{σ} for each single drive problem has been found. These functions are solutions of the linearized drift kinetic equation (3.22).

Finally, the full set of relations between the flux surface averaged thermodynamic radial fluxes and forces may be represented as

$$\begin{pmatrix}
\langle \Gamma_e^r \rangle \\
\frac{\langle Q_e^r \rangle}{T_e} \\
-\frac{\langle j_{\parallel} \hat{B} \rangle}{e}
\end{pmatrix} = - \begin{pmatrix}
L_{11}^e & L_{12}^e & L_{13}^e \\
L_{21}^e & L_{22}^e & L_{23}^e \\
L_{31}^e & L_{32}^e & L_{33}^e
\end{pmatrix} \begin{pmatrix}
A_1^e \\
A_2^e \\
A_3^e
\end{pmatrix},$$
(3.46)

with

$$A_1^e(r) = \left(\frac{1}{n_e} \frac{\partial n_e}{\partial \psi} - \frac{3}{2T_e} \frac{\partial T_e}{\partial \psi} - \frac{e}{T_e} \frac{\partial \Phi}{\partial \psi}\right) \langle |\nabla \psi| \rangle \tag{3.47}$$

$$A_2^e(r) = \left(\frac{1}{T_e} \frac{\partial T_e}{\partial \psi}\right) \langle |\nabla \psi| \rangle \tag{3.48}$$

$$A_3^e(r) = -\frac{e}{T_e} \frac{\langle E_{\parallel}^{(A)} \hat{B} \rangle}{\langle \hat{B}^2 \rangle}. \tag{3.49}$$

3.2.1 Thermal transport coefficients

Upon inserting the expansion of the normalized distribution function,

$$\hat{f}_{k}^{\sigma}(\psi, s, x, \lambda) = f_{e0}(\psi, x) \sum_{m} f_{m}^{\sigma,(k)}(\psi, s, \lambda) \varphi_{m}(x)
= \frac{n_{e}}{\pi^{3/2} v_{te}^{3}} e^{-x^{2}} \sum_{m} f_{m}^{\sigma,(k)}(\psi, s, \lambda) \varphi_{m}(x) , \qquad (3.50)$$

into Eq. (3.45), one can perform the integration with respect to normalized speed. This yields the expression for the thermal transport coefficients, namely,

$$L_{jk}^{e} = \frac{n_{e}}{\tau_{ee}} l_{c} \beta_{j} \beta_{k} \sum_{m} \sum_{\sigma=\pm 1} b_{m}^{(j)} \left\langle \frac{\hat{B}}{4} \int_{0}^{1/\hat{B}} d\eta q_{j}^{-\sigma} f_{m}^{\sigma,(k)} \right\rangle , \qquad (3.51)$$

with

$$b_m^{(j)} \equiv 4\pi \left(\varphi_m, x^{2(j-1)-5\delta_{3j}}\right)$$

$$= \frac{4}{\sqrt{\pi}} \int_0^\infty dx e^{-x^2} x^{2(j+1)-5\delta_{3j}} \varphi_m(x) , \qquad (3.52)$$

for j = 1, 2, 3 representing numerical coefficients independent of problem parameters. These quantities are given by

$$b_m^{(1)} = \frac{4}{\sqrt{\pi}} \int_0^\infty dx \, e^{-x^2} x^4 \varphi_m(x) = \sqrt{6\pi} \delta_{m0}, \qquad (3.53)$$

$$b_m^{(2)} = \frac{4}{\sqrt{\pi}} \int_0^\infty dx \, e^{-x^2} x^6 \varphi_m(x) = \frac{5\sqrt{6\pi}}{2} \delta_{m0} - \sqrt{15\pi} \delta_{m1}, \tag{3.54}$$

$$b_m^{(3)} = \frac{4}{\sqrt{\pi}} \int_0^\infty dx \, e^{-x^2} x^3 \varphi_m(x) = \left[\frac{32}{\sqrt{\pi}} \frac{\Gamma(m+1/2)}{m!(2m+1)(2m+3)} \right]^{1/2}. (3.55)$$

Here, Eq. (3.55) may be calculated using the following recurrence relation,

$$b_{m+1}^{(3)} = b_m^{(3)} \frac{(m+1/2)}{\sqrt{(m+1)(m+5/2)}},$$
(3.56)

with initial value $b_0^{(3)} = 4\sqrt{2/3}$.

It is convenient to define the dimensionless transport coefficients γ_{jk} , which depend only on the device geometry, the mean free path l_c and the effective charge Z_{eff} ,

$$\gamma_{jk} = \frac{\alpha_j \alpha_k}{l_c} \sum_{m} \sum_{\sigma = \pm 1} b_m^{(j)} \left\langle \frac{\hat{B}}{4} \int_0^{1/\hat{B}} d\eta q_j^{-\sigma} f_m^{\sigma,(k)} \right\rangle , \qquad (3.57)$$

with

$$\alpha_1 = \alpha_2 = \frac{l_c}{\langle |\nabla \psi| \rangle}, \qquad \alpha_3 = 1,$$
(3.58)

and

$$\hat{\beta}_1 = \hat{\beta}_2 = \rho_{e0} , \qquad \hat{\beta}_3 = l_c , \qquad (3.59)$$

respectively. Hence, the dimensional electron transport matrix, Eq. (3.51), reads

$$L_{jk}^{e} = \frac{n_e}{\tau_{ee}} \hat{\beta}_j \hat{\beta}_k \gamma_{jk}. \tag{3.60}$$

It should be noted that the transport matrices L_{jk}^e and γ_{jk} correspond to the effective radius r used as a radial variable where dr = dV/S, V is a volume limited by a flux surface and S is a flux surface area. In order to obtain these matrices for different definitions of plasma radius, e.g., for the radius defined via the toroidal flux ψ , $r_{\psi} = (2\psi/B_{00})^{1/2}$, coefficients α_1 and α_2 should be multiplied by dr_{ψ}/dr . The quantity B_{00} denotes the amplitude of the (0,0) magnetic field harmonic in Boozer coordinates.

3.2.2 Monoenergetic transport coefficients

By neglecting in Eq. (3.22) energy scattering as well as momentum conservation one may obtain the monoenergetic transport coefficients $L_{jk}^{e,\text{mono}}$. After substituting into Eq. (3.45) the normalized functions \tilde{f}_k^{σ} ,

$$\hat{f}_k^{\sigma} = x^{2k-1-5\delta_{3k}} f_{e0} \tilde{f}_k^{\sigma}$$
, for $k = 1, 2, 3$ (3.61)

and replacing the Maxwellian distribution function by $n_e \delta(x-x_0)/(4\pi v_{te}^3 x_0^2)$ one obtains

$$L_{jk}^{e,\text{mono}} = \frac{n_e v_{te} \beta_j \beta_k}{x_0^2} \int_0^\infty dx x^{\zeta(j,k)+2} \delta(x-x_0) \sum_{\sigma=\pm 1} \left\langle \frac{\hat{B}}{4} \int_0^{1/B} d\eta q_j^{-\sigma} \tilde{f}_k^{\sigma} \right\rangle$$

$$= n_e v_{te} \beta_j \beta_k x_0^{\zeta(j,k)} \sum_{\sigma=\pm 1} \left\langle \frac{\hat{B}}{4} \int_0^{1/\hat{B}} d\eta q_j^{-\sigma} \tilde{f}_k^{\sigma} \right\rangle$$

$$= n_e D_{jk}^{\text{mono}}, \qquad (3.62)$$

with β_j introduced in Eq. (3.18). The monoenergetic transport coefficients have been defined by

$$D_{jk}^{\text{mono}} \equiv v_{te} \beta_j \beta_k x_0^{\zeta(j,k)} \sum_{\sigma=\pm 1} \left\langle \frac{\hat{B}}{4} \int_0^{1/\hat{B}} d\eta q_j^{-\sigma}(\eta) \tilde{f}_k^{\sigma}(x_0, \eta) \right\rangle, \tag{3.63}$$

where the abbreviation

$$\zeta(j,k) = 2(j+k) - 1 - 5(\delta_{3j} + \delta_{3k}) \tag{3.64}$$

has been used. Note that the monoenergetic transport coefficients depend on the deflection frequency ν_D^e , or strictly speaking,

$$D_{jk}^{\text{mono}} = D_{jk}^{\text{mono}}(\nu_D^e(v)/v). \tag{3.65}$$

3.2.3 Energy convolution

For the case when only pitch-angle scattering is assumed the elements of the thermal transport matrix can be calculated from the convolution of the Maxwellian distribution function with monoenergetic coefficients [32], $D_{jk}^{\text{mono}}(v)$, that have been obtained in Chapter 3.2.2. From Eqs. (3.45) and (3.61), by using Eq. (3.63), it follows that

$$L_{jk}^{e,\mathcal{L}} = 4\pi v_{te}^{4} \beta_{j} \beta_{k} \int_{0}^{\infty} dx x^{\zeta(j,k)+2} f_{e0}(x) \sum_{\sigma=\pm 1} \left\langle \frac{\hat{B}}{4} \int_{0}^{1/\hat{B}} d\eta q_{j}^{-\sigma} \tilde{f}_{k}^{\sigma}(x,\eta) \right\rangle$$

$$= 4\pi v_{te}^{3} \int_{0}^{\infty} dx x^{2} f_{e0}(x) D_{jk}^{\text{mono}}(x)$$

$$= \frac{4n_{e}}{\sqrt{\pi}} \int_{0}^{\infty} dx e^{-x^{2}} x^{2} D_{jk}^{\text{mono}}(x). \tag{3.66}$$

Recalling Eq. (3.60), the corresponding dimensionless coefficients are given by

$$\gamma_{jk}^{\mathcal{L}} = \frac{4l_c}{\sqrt{\pi}\hat{\beta}_j\hat{\beta}_k v_{te}} \int_0^\infty \mathrm{d}x e^{-x^2} x^2 D_{jk}^{\text{mono}}(x). \tag{3.67}$$

It has to be noted that the collisionality parameter in the monoenergetic case, $\kappa^{\text{mono}} = \nu_D^e(v)/v$, is different from the one of Eq. (3.26), $\kappa = 1/(v_{te}\tau_{ee})$, where

the full linearized collision operator has been applied (see Chapter 3.1). The connection between these quantities is as follows,

$$\kappa^{\text{mono}} = \kappa \frac{v_{te} \tau_{ee}}{v} \nu_D^e(v) \qquad (3.68)$$

$$= \kappa \frac{v_{te} \tau_{ee}}{v} \left(\nu_D^{ee} + \sum_{s \neq e} \nu_D^{es} \right)$$

$$= \kappa \alpha(x, Z). \qquad (3.69)$$

The function α is defined by

$$\alpha \equiv \frac{\tau_{ee}}{x} \left[\nu_D^{ee}(v) + \sum_{s \neq e} \nu_D^{es}(v) \right], \tag{3.70}$$

with the deflection frequencies of electron and background ions,

$$\tau_{ee}\nu_D^{ee} = \frac{3\sqrt{\pi}}{4} \frac{[\phi(x) - G(x)]}{x^3} ,$$
(3.71)

$$\tau_{ee}\nu_D^{es} = \frac{3\sqrt{\pi}}{4} \frac{Z_s^2 n_s}{n_e} \frac{[\phi(y) - G(y)]}{x^3}.$$
(3.72)

Here, $x = v/v_{te}$, $y = v/v_{ts}$, $\phi(y)$ denotes the error function

$$\phi(y) \equiv \frac{2}{\sqrt{\pi}} \int_0^y \mathrm{d}t e^{-t^2},\tag{3.73}$$

and G(y) is the so-called Chandrasekhar function [22]

$$G(y) \equiv \frac{\phi(y) - y\phi'(y)}{2y^2},\tag{3.74}$$

where the prime indicates a derivative with respect to the argument.

Assuming infinitely heavy background ions one obtains for Eq. (3.72)

$$\tau_{ee}\nu_D^{e\infty} = \frac{3\sqrt{\pi}}{4} \frac{Z_s^2 n_s}{n_e x^3}.$$
 (3.75)

Thus, the relation between the collisionality parameters κ^{mono} and κ can be expressed as

$$\kappa^{\text{mono}} = \kappa \alpha(x, Z_{\text{eff}}),$$
(3.76)

with function

$$\alpha(x, Z_{\text{eff}}) = \frac{3\sqrt{\pi}}{4x^4} \left[\phi(x) - G(x) + Z_{\text{eff}} \right], \tag{3.77}$$

and

$$Z_{\text{eff}} = \frac{\sum_{s} Z_s^2 n_s}{n_e},\tag{3.78}$$

respectively. The sum in the last equation is taken over all ion species s.

3.2.4 Onsager symmetry

The proof of the Onsager symmetry [33] (which is a consequence of the self-adjointness property of the collision operator [23]) of the transport coefficients follows References 34 and 35, respectively. From Eq. (3.22) one gets the following equations

$$v|\lambda|\frac{\partial f_j^+}{\partial s} - \mathcal{C}_e^l[f_j^+] = f_{e0}Q_j^+$$
(3.79)

$$-v|\lambda|\frac{\partial f_j^-}{\partial s} - \mathcal{C}_e^l[f_j^-] = f_{e0}Q_j^-. \tag{3.80}$$

Introducing for any function $F(\mathbf{v})$ its even and odd part with respect to σ , that is

$$F^{\text{even}} \equiv \frac{1}{2} \sum_{\sigma' = +1} F^{\sigma'} = \frac{1}{2} \left(F^+ + F^- \right)$$
 (3.81)

$$F^{\text{odd}} \equiv \frac{1}{2} \sum_{\sigma'=+1} \sigma' F^{\sigma'} = \frac{1}{2} \left(F^+ - F^- \right) ,$$
 (3.82)

one obtains from Eqs. (3.79) and (3.80),

$$v|\lambda|\frac{\partial f_j^{\text{odd}}}{\partial s} - \mathcal{C}_e^l[f_j^{\text{even}}] = f_{e0}Q_j^{\text{even}}$$
 (3.83)

$$v|\lambda| \frac{\partial f_k^{\text{even}}}{\partial s} - \mathcal{C}_e^l[f_k^{\text{odd}}] = f_{e0}Q_k^{\text{odd}}, \qquad (3.84)$$

whereupon in the last equation the index j has been changed to k. Now, multiplying Eq. (3.83) by f_k^{even}/f_{e0} and Eq. (3.84) by f_j^{odd}/f_{e0} , integrating both equations over velocity space and averaging over a magnetic surface one arrives at the relations

$$\left\langle \int d^3 v v |\lambda| \frac{f_k^{\text{even}}}{f_{e0}} \frac{\partial f_j^{\text{odd}}}{\partial s} \right\rangle - \left\langle \int d^3 v \frac{f_k^{\text{even}}}{f_{e0}} C_e^l [f_j^{\text{even}}] \right\rangle$$

$$= \left\langle \int d^3 v Q_j^{\text{even}} f_k^{\text{even}} \right\rangle \qquad (3.85)$$

$$\left\langle \int d^3 v v |\lambda| \frac{f_j^{\text{odd}}}{f_{e0}} \frac{\partial f_k^{\text{even}}}{\partial s} \right\rangle - \left\langle \int d^3 v \frac{f_j^{\text{odd}}}{f_{e0}} C_e^l [f_k^{\text{odd}}] \right\rangle$$

$$= \left\langle \int d^3 v Q_k^{\text{odd}} f_j^{\text{odd}} \right\rangle. \tag{3.86}$$

Taking into account that

$$Q_1^{\text{odd}} = Q_2^{\text{odd}} = 0 (3.87)$$

$$Q_3^{\text{even}} = 0,$$
 (3.88)

it can be shown that the RHS of Eqs. (3.85) and (3.86) are equal to the transport coefficients, that is

$$\left\langle \int d^3 v Q_j^{\text{even}} f_k^{\text{even}} \right\rangle = (\delta_{1j} + \delta_{2j}) L_{jk}^e , \qquad (3.89)$$

and

$$\left\langle \int d^3 v Q_k^{\text{odd}} f_j^{\text{odd}} \right\rangle = -\delta_{3k} L_{kj}^e , \qquad (3.90)$$

respectively. Due to the self-adjoint property of the linearized collision operator (see, e.g., [36]),

$$\int d^3 v \frac{g}{f_{e0}} C_e^l[h] = \int d^3 v \frac{h}{f_{e0}} C_e^l[g]$$
(3.91)

and upon using the antisymmetry relation

$$\left\langle \int d^3 v g v_{\parallel} \frac{\partial h}{\partial s} \right\rangle = -\left\langle \int d^3 v h v_{\parallel} \frac{\partial g}{\partial s} \right\rangle, \tag{3.92}$$

for the first term on the LHS of Eqs. (3.85) and (3.86), respectively, one obtains the Onsager symmetry for the electron transport matrix L_{jk}^{e} in the form

$$(\delta_{1j} + \delta_{2j} + \delta_{3j})L_{jk}^e = (\delta_{1k} + \delta_{2k} + \delta_{3k})L_{kj}^e, \tag{3.93}$$

and

$$L_{12}^e = L_{21}^e (3.94)$$

$$L_{13}^e = L_{31}^e (3.95)$$

$$L_{23}^e = L_{32}^e, (3.96)$$

accordingly.

3.3 Fluxes and forces

Here, it is worth noting that the choice of neoclassical fluxes and thermodynamical forces is not unique [23,37] and, consequently, giving rise to differing transport matrices. In this work the fluxes have been chosen to be the surface averaged total radial fluxes of particles, $\langle \Gamma_a^r \rangle$, and energy, $\langle Q_a^r \rangle$, as well as the surface averaged total parallel current density $\langle j_{\parallel} \hat{B} \rangle$ [cf. definitions in Eqs. (3.37)-(3.39), respectively]. In the literature, however, the second flux is often defined by means of the flux surface averaged radial heat flux $\langle q_a^r \rangle$

(see, e.g., References 28 and 38), which is connected to the energy flux by the relation

$$\langle Q_a^r \rangle = \frac{5}{2} T_a \langle \Gamma_a^r \rangle + \langle q_a^r \rangle,$$
 (3.97)

where the first part on the RHS of Eq. (3.97) represents the convective energy flux. From this it follows, that the set of fluxes can be written as

$$I_1' = I_1 (3.98)$$

$$I_{2}^{'} = I_{2} - \frac{5}{2}I_{1} \tag{3.99}$$

$$I_3' = I_3, (3.100)$$

which may also be expressed in terms of a transformation matrix, that is

$$\mathbf{I}' = \mathbf{M} \cdot \mathbf{I}, \qquad \mathbf{M}_{jk} = \begin{pmatrix} 1 & 0 & 0 \\ \alpha & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$
 (3.101)

with $\alpha = -5/2$ and where matrix notation has been used. This new set of fluxes requires the modification of the driving forces as well. If the matrix **L**, defined via the fluxes **I** and forces **A** [cf. Eq. (3.42)], is symmetric and the new matrix \mathbf{L}' is defined by means of the new fluxes and forces, \mathbf{I}' and \mathbf{A}' , respectively, such that $I_1' = I_1$, $I_2' = \alpha I_1 + I_2$ and $I_3' = I_3$, freedom in definition of the new forces \mathbf{A}' as linear combinations of old forces \mathbf{A} is limited to a scaling constant C, namely,

$$A_{1}^{'} = C(A_{1} - \alpha A_{2})$$
 (3.102)
 $A_{2}^{'} = CA_{2}$ (3.103)

$$A_2' = CA_2 (3.103)$$

$$A_3^{'} = CA_3. ag{3.104}$$

This transformation is obtained from the conditions that \mathbf{L}' is symmetric and transformation coefficients from A to A' are independent of L. Here, the arbitrary constant C is fixed to 1, which leads to

$$A_{1}^{'} = \left(\frac{1}{n_{a}T_{a}}\frac{\partial n_{a}T_{a}}{\partial \psi} + \frac{e_{a}}{T_{a}}\frac{\partial \Phi}{\partial \psi}\right) \langle |\nabla \psi| \rangle. \tag{3.105}$$

Furthermore, by using Eqs. (3.42) and (3.101) one obtains

$$\mathbf{I}' = \mathbf{M} \cdot \mathbf{I}$$

$$= -\mathbf{M} \cdot (\mathbf{L} \cdot \mathbf{A})$$

$$= -(\mathbf{M} \cdot \mathbf{L}) \cdot (\mathbf{M}^T \cdot \mathbf{A}')$$

$$= -(\mathbf{M} \cdot \mathbf{L} \cdot \mathbf{M}^T) \cdot \mathbf{A}', \qquad (3.106)$$

where $\mathbf{A} = \mathbf{M}^T \cdot \mathbf{A}'$ has been calculated from Eqs. (3.102)-(3.104). Therefore, the new neoclassical transport matrix is given by

$$\mathbf{L}' = \mathbf{M} \cdot \mathbf{L} \cdot \mathbf{M}^T, \tag{3.107}$$

from which it follows that

$$L_{11}^{'} = L_{11} \tag{3.108}$$

$$L'_{12} = L_{12} - \frac{5}{2}L_{11} = L'_{21}$$
 (3.109)

$$L_{13}^{'} = L_{13} = L_{31}^{'} (3.110)$$

$$L'_{13} = L_{13} = L'_{31}$$

$$L'_{22} = L_{22} - 5L_{12} + \frac{25}{4}L_{11}$$
(3.110)

$$L'_{23} = L_{23} - \frac{5}{2}L_{13} = L'_{32}$$
 (3.112)

$$L'_{33} = L_{33}, (3.113)$$

where Onsager symmetry has been applied [cf. Eqs. (3.94)-(3.96)].

Chapter 4

Generalized Spitzer function

The standard method for calculation of electron cyclotron current drive (ECCD) generated current in tokamaks and stellarators is the adjoint approach where the flux surface averaged current is given by a convolution of a quasilinear source term with the adjoint generalized Spitzer function (local current drive efficiency). This function is well studied for high collisionality regimes where it is equivalent to the classical Spitzer function [39], and in the long mean free path (LMFP) regime where a bounce averaging procedure can be used to reduce the dimensionality of the problem to 2D. For a detailed discussion of various approaches to the LMFP regime see Reference 40. For benchmarking results of various codes and pertinent models especially for ITER see References 41,42 and citations within these papers.

In the general case of finite plasma collisionality, the kinetic problem to compute the local efficiency remains essentially 3D for tokamaks and 4D for stellarators. For this reason, this general case is not studied as well as cases in the asymptotic limits [43].

In the linear approximation, generation of steady state plasma current by ECCD is described by the linearized kinetic equation

$$v_{\parallel} \mathbf{h} \cdot \nabla \tilde{f} - \mathcal{C}^{l}[\tilde{f}] = Q_{RF}, \tag{4.1}$$

where \tilde{f} is the perturbation of the electron distribution function, **h** is a unit vector along the magnetic field, v_{\parallel} is the parallel velocity, C^{l} represents the full linearized collision integral and Q_{RF} is a quasilinear particle source in the phase space.

By means of the adjoint approach (which allows one to compute the current density without having to find \tilde{f} , see, e.g., Reference 44) the flux surface

A large part of this chapter has already been published in: W. Kernbichler, S. V. Kasilov, G. O. Leitold, V. V. Nemov and N. B. Marushchenko, *Generalized Spitzer Function with Finite Collisionality in Toroidal Plasmas*, Contrib. Plasma Phys. **50**, 761 (2010).

averaged parallel current density may be calculated via the adjoint generalized Spitzer function \bar{g} (current drive efficiency), which is expressed through the generalized Spitzer function g as follows, $\bar{g}(v_{\parallel}) = g(-v_{\parallel})$, where $g(v_{\parallel})$ is the solution to the conductivity problem,

$$v_{\parallel} \mathbf{h} \cdot \nabla f_M g - \mathcal{C}^l[f_M g] = \frac{1}{l_{\text{Sp}}} v_{\parallel} f_M, \tag{4.2}$$

and f_M is a Maxwellian. Here, Eq. (4.2) represents a generalization of the collisional Spitzer problem [39, 45]. This equation may be recast to give

$$v_{\parallel} \mathbf{h} \cdot \nabla f_M \bar{g} + \mathcal{C}^l[f_M \bar{g}] = \frac{1}{l_{\rm Sp}} v_{\parallel} f_M. \tag{4.3}$$

Upon substitution of the RHS of Eq. (4.3) into the definition for the flux surface averaged current density

$$\langle j_{\parallel} \rangle = e \left\langle \int d^3 p \ v_{\parallel} \tilde{f} \right\rangle,$$
 (4.4)

it follows that

$$\langle j_{\parallel} \rangle = e \, l_{\rm Sp} \left\langle \int d^{3}p \, \frac{\tilde{f}}{f_{M}} \frac{v_{\parallel} f_{M}}{l_{\rm Sp}} \right\rangle$$

$$= e \, l_{\rm Sp} \left\langle \int d^{3}p \, \frac{\tilde{f}}{f_{M}} \Big(v_{\parallel} \mathbf{h} \cdot \nabla f_{M} \bar{g} + \mathcal{C}^{l}[f_{M} \bar{g}] \Big) \right\rangle$$

$$= e \, l_{\rm Sp} \left\langle \int d^{3}p \, \bar{g} \left(-v_{\parallel} \mathbf{h} \cdot \nabla \tilde{f} + \mathcal{C}^{l}[\tilde{f}] \right) \right\rangle, \tag{4.5}$$

where the antisymmetry relation

$$\left\langle \int d^3 p \, F v_{\parallel} \frac{\partial G}{\partial s} \right\rangle = -\left\langle \int d^3 p \, G v_{\parallel} \frac{\partial F}{\partial s} \right\rangle,\tag{4.6}$$

as well as the self-adjoint property of the collision operator,

$$\int d^3p \ F \mathcal{C}^l[f_M G] = \int d^3p \ G \mathcal{C}^l[f_M F], \tag{4.7}$$

has been utilized. Finally, from Eqs. (4.5) and (4.1) one obtains for the flux surface averaged parallel current density

$$\langle j_{\parallel} \rangle = -e \, l_{\rm Sp} \left\langle \int \mathrm{d}^3 p \, \bar{g} \, Q_{RF} \right\rangle,$$
 (4.8)

where p is the momentum, $\langle ... \rangle$ denotes the flux surface average [average over the volume between neighboring flux surfaces, see Eq. (3.12)], e is electron charge, $l_{\rm Sp}$ is the free path length given by $l_{\rm Sp} = T_e^2/(\pi n_e e^4 \ln \Lambda)$ where n_e , T_e and $\ln \Lambda$ are electron density, temperature and Coulomb logarithm, respectively.

Using a more explicit form for the quasilinear source term,

$$Q_{RF} = -\frac{\partial}{\partial \mathbf{p}} \cdot \mathbf{\Gamma}_{RF},\tag{4.9}$$

the parallel current density is expressed via derivatives of the adjoint Spitzer function

$$\langle j_{\parallel} \rangle = -e \, l_{\rm Sp} \left\langle \int \mathrm{d}^3 p \, \frac{\partial \bar{g}}{\partial \mathbf{p}} \cdot \mathbf{\Gamma}_{RF} \right\rangle.$$
 (4.10)

Here, Γ_{RF} is the momentum space flux density due to the wave-induced quasilinear diffusion.

Within geometrical optics used for calculation of ECRH/ECCD, quasilinear flux density can be described in local approximation. In this approximation Γ_{RF} differs from zero in the velocity space only at the resonance line where the (multiple) cyclotron resonance condition taking into account Doppler shift is fulfilled, $\omega = n\omega_c + k_{\parallel}v_{\parallel}$, where ω , ω_c , n and k_{\parallel} are wave frequency, relativistic (energy dependent) cyclotron frequency, cyclotron harmonic index and parallel wave vector, respectively. For weakly relativistic electrons these resonance lines are close to circles on the $(p_{\perp}, p_{\parallel})$ plane whose centers are located at $p_{\perp} = 0$ axis. In this weakly relativistic case, the largest component of the quasilinear flux density is over perpendicular momentum. Therefore, as follows from Eq. (4.10), the behavior of the derivative of \bar{g} over perpendicular momentum at the resonance curve is of main importance for ECCD.

In the code NEO-2, the dependence of the generalized Spitzer function on kinetic energy is presented in the form of expansion over the associated Laguerre polynomials of the order 3/2 (Sonine polynomials),

$$g(\mathbf{r}, \mathbf{p}) = \sum_{m=0}^{M} g_m(\mathbf{r}, \eta) L_m^{(3/2)} \left(\frac{p^2}{2m_e T_e}\right).$$
 (4.11)

The expansion coefficients g_m are discretized on the adaptive grid over η which reduces the kinetic equation (4.2) to a set of coupled ordinary differential equations with the independent variable being the distance counted along the field line (cf. Chapter 3.1). This set of equations is solved by numerical ODE integration (see Reference 46 for details).

Chapter 5

Calculation of the matrix elements

In Chapter 3 the derivation of the transformed drift kinetic equation [see Eq. (3.26)] to be numerically solved by means of the NEO-2 code (see, e.g., References 25 and 46) has been presented without going into mathematical details. In the following, this equation will be derived explicitly and the matrix elements (moments of the Coulomb collision operator) arising will be evaluated.

A solution to the drift kinetic equation for a single-drive problem [see Eq. (3.22) in Chapter 3.1]

$$\sigma v |\lambda| \frac{\partial \hat{f}_k^{\sigma}}{\partial s} - \mathcal{C}_a^l [\hat{f}_k^{\sigma}] = f_{a0} v_{ta} x^{2k - 5\delta_{3k}} |\lambda| q_k^{\sigma} , \qquad \text{for} \quad k = 1, 2, 3$$
 (5.1)

is obtained upon the substitution of the truncated series approximation for the distribution function,

$$\hat{f}_k^{\sigma}(\psi, s, x, \lambda) \approx f_{a0}(\psi, x) \sum_{m'=0}^{M} f_{m'}^{\sigma,(k)}(\psi, s, \lambda) \varphi_{m'}(x)$$
 (5.2)

into Eq. (5.1), where the test functions φ_m are defined as

$$\varphi_m(x) \equiv \frac{\pi^{3/4}}{\sqrt{h_m}} L_m^{(3/2)}(x^2), \quad \text{for} \quad m = 0, 1, 2, \dots, M,$$
(5.3)

and $h_m = \Gamma(m + 5/2)/(2m!)$ denotes the normalization factor (see Appendix A.1). This leads to the following equation,

$$\sum_{m'=0}^{M} \left(\sigma v f_{a0} \varphi_{m'} |\lambda| \frac{\partial f_{m'}^{\sigma,(k)}}{\partial s} - \mathcal{C}_a^l \left[f_{a0} f_{m'}^{\sigma,(k)} \varphi_{m'} \right] \right) = f_{a0} v_{ta} x^{2k-5\delta_{3k}} |\lambda| q_k^{\sigma} , \quad (5.4)$$

where \mathcal{C}_a^l is the linearized Coulomb collision operator

$$C_a^l[f_m] = \sum_b \left(C_{ab}[f_m, f_{b0}] + C_{ab}[f_{a0}, f_m] \right)$$
(5.5)

comprising a differential and an integral part, respectively (for details see Appendix B) and where the expansion coefficients $f_m^{\sigma,(k)}$ are to be determined. The matrix elements are calculated from Eq. (5.4) upon multiplication on the left by the basis function φ_m followed by an integration over $(n_a v_{ta}^2)^{-1} \int_0^\infty dv v^3$. One obtains for the first term on the LHS of Eq. (5.4)

$$\frac{1}{n_{a}v_{ta}^{2}} \int_{0}^{\infty} dv v^{3} \varphi_{m} \sum_{m'=0}^{M} \sigma v f_{a0} \varphi_{m'} |\lambda| \frac{\partial f_{m'}^{\sigma,(k)}}{\partial s}
= \sum_{m'=0}^{M} \sigma |\lambda| \frac{\partial f_{m'}^{\sigma,(k)}}{\partial s} \frac{1}{n_{a}v_{ta}^{2}} \int_{0}^{\infty} dv v^{4} f_{a0} \varphi_{m} \varphi_{m'}
= \sum_{m'=0}^{M} \sigma |\lambda| \frac{\partial f_{m'}^{\sigma,(k)}}{\partial s} (\varphi_{m}, \varphi_{m'})
= \sigma |\lambda| \frac{\partial f_{m}^{\sigma,(k)}}{\partial s},$$
(5.6)

where the orthonormalization relation for the basis functions φ_m ,

$$(\varphi_m, \varphi_{m'}) = \delta_{mm'}, \tag{5.7}$$

has been used (see Appendix A). The evaluation of the other parts of Eq. (5.4) is somewhat more involved and will be carried out in the following chapters.

5.1 Source term

Performing the same steps as described above the RHS of Eq. (5.1) can be transformed to

$$\frac{1}{n_{a}v_{ta}^{2}} \int_{0}^{\infty} dv v^{3} \varphi_{m} f_{a0} v_{ta} x^{2k-5\delta_{3k}} |\lambda| q_{k}^{\sigma}$$

$$= |\lambda| q_{k}^{\sigma} \frac{1}{n_{a}v_{ta}^{2}} \int_{0}^{\infty} dv v^{4} \frac{1}{x} \varphi_{m} f_{a0} x^{2k-5\delta_{3k}}$$

$$= |\lambda| q_{k}^{\sigma} a_{m}^{(k)}, \qquad (5.8)$$

where the abbreviation

$$a_m^{(k)} \equiv \left(\varphi_m, x^{2k-1-5\delta_{3k}}\right) \tag{5.9}$$

has been introduced. The scalar product between a test function φ_m and an arbitrary integer power of normalized speed x can be carried out, yielding

$$(\varphi_m, x^j) = \frac{1}{n_a v_{ta}^2} \int_0^\infty dv v^4 f_{a0}(x) \varphi_m(x) x^j$$

$$= \frac{1}{\pi^{3/4} \sqrt{h_m}} \int_0^\infty dx e^{-x^2} x^{j+4} L_m^{(3/2)}(x^2)$$

$$= \frac{1}{\pi^{3/4}} \left[\frac{2m!}{\Gamma(m+5/2)} \right]^{1/2} \frac{\Gamma[(j+5)/2]\Gamma(m-j/2)}{2m!\Gamma(-j/2)} , \quad (5.10)$$

where

$$\int_{0}^{\infty} dt e^{-t} t^{\gamma - 1} L_m^{(\mu)}(t) = \frac{\Gamma(\gamma)\Gamma(m + \mu - \gamma + 1)}{m!\Gamma(\mu - \gamma + 1)}, \quad \text{Re } \gamma > 0$$
 (5.11)

has been used [29]. The quantities $a_m^{(k)}$ for k = 1, 2, 3 can now be evaluated by means of Eq. (5.10) giving the results

$$a_m^{(1)} \equiv (\varphi_m, x) = \frac{1}{\pi^{3/4}} \left[\frac{2m!}{\Gamma(m+5/2)} \right]^{1/2} \frac{\Gamma(3)\Gamma(m-1/2)}{2m!\Gamma(-1/2)}$$
$$= -\frac{\Gamma(m-1/2)}{\pi^{5/4} \left[2m!\Gamma(m+5/2) \right]^{1/2}}, \tag{5.12}$$

$$a_m^{(2)} \equiv (\varphi_m, x^3) = \frac{1}{\pi^{3/4}} \left[\frac{2m!}{\Gamma(m+5/2)} \right]^{1/2} \frac{\Gamma(4)\Gamma(m-3/2)}{2m!\Gamma(-3/2)}$$

$$= \frac{9\Gamma(m-3/2)}{2\pi^{5/4} \left[2m!\Gamma(m+5/2) \right]^{1/2}}$$

$$= -\frac{9}{(2m-3)} a_m^{(1)}, \qquad (5.14)$$

$$a_m^{(3)} \equiv (\varphi_m, 1) = \frac{1}{2} \sqrt{\frac{3}{2\pi}} (\varphi_m, \varphi_0)$$

= $\frac{1}{2} \sqrt{\frac{3}{2\pi}} \delta_{m0},$ (5.15)

whereas in the last equation the orthonormalization relation for the functions φ_m has been utilized [cf. Eq. (5.7)].

5.2 Differential part of the collision operator

The test particle part of the Coulomb collision operator has the representation (see, e.g., Reference 22 or Appendix B.4.2)

$$C_{ab}[f_m, f_{b0}] = \nu_D^{ab}(v) \mathcal{L}[f_m] + C_{ab}^{D,v}[f_m], \qquad (5.16)$$

with \mathcal{L} denoting the pitch-angle scattering operator [see Eq. (B.87)] and where $\mathcal{C}_{ab}^{D,v}$ accounts for energy scattering. The latter term is given by

$$C_{ab}^{D,v}[f_m] = \frac{1}{v^2} \frac{\partial}{\partial v} \left[v^3 \left(\frac{m_a}{m_a + m_b} \nu_s^{ab}(v) f_m + \frac{1}{2} \nu_{\parallel}^{ab}(v) v \frac{\partial f_m}{\partial v} \right) \right]. \tag{5.17}$$

The collision frequencies appearing in Eqs. (5.16) and (5.17) are defined by [22]

$$\nu_D^{ab}(v) = \hat{\nu}_{ab} \frac{\phi(y) - G(y)}{x^3},\tag{5.18}$$

where $\hat{\nu}_{ab} = 3\sqrt{\pi}/(4\tau_{ab})$, $x = v/v_{ta}$, $y = v/v_{tb} = \gamma_{ab}x$, and $\gamma_{ab} = v_{ta}/v_{tb}$, and by

$$\nu_s^{ab}(v) = \hat{\nu}_{ab} \frac{2T_a}{T_b} \left(1 + \frac{m_b}{m_a} \right) \frac{G(y)}{x}$$
 (5.19)

$$\nu_{\parallel}^{ab}(v) = 2\hat{\nu}_{ab} \frac{G(y)}{x^3}, \tag{5.20}$$

respectively, designating the deflection frequency, the slowing down frequency and the parallel velocity diffusion frequency. The quantity

$$G(y) = \frac{\phi(y) - y\phi'(y)}{2y^2}$$
 (5.21)

is the so-called Chandrasekhar function [22].

5.2.1 Lorentz part of $C_{ab}[f_{a1}, f_{b0}]$

Applying the same operations as those used for obtaining Eqs. (5.4) and (5.6), respectively, to the Lorentz part of the test particle operator [cf. Eq. (5.16)] one gets

$$\frac{1}{n_a v_{ta}^2} \int_0^\infty dv v^3 \varphi_m \sum_{m'=0}^M \sum_b \nu_D^{ab}(v) \mathcal{L} \left[f_{a0} f_{m'}^{\sigma,(k)} \varphi_{m'} \right]$$

$$= \sum_{m'=0}^{M} \sum_{b} \left(\frac{1}{n_a v_{ta}^2} \int_{0}^{\infty} dv v^3 f_{a0} \varphi_m \nu_D^{ab} \varphi_{m'} \right) \mathcal{L} \left[f_{m'}^{\sigma,(k)} \right]$$

$$= \kappa \sum_{m'=0}^{M} \sum_{b} \nu_{mm'}^{ab} \mathcal{L} \left[f_{m'}^{\sigma,(k)} \right], \qquad (5.22)$$

where the collisionality parameter $\kappa \equiv 1/(v_{ta}\tau_{aa})$ and $\nu_{mm'}^{ab}$ denotes the matrix elements of the Lorentz operator defined as

$$\nu_{mm'}^{ab} \equiv v_{ta} \tau_{aa} \left(\varphi_m \left| v^{-1} \nu_D^{ab} \right| \varphi_{m'} \right). \tag{5.23}$$

Employing the definitions of the test functions φ_m , Eq. (5.3), as well as the relation for the deflection frequency ν_D^{ab} , Eq. (5.18), it follows from Eq. (5.23) that

$$\nu_{mm'}^{ab} = \frac{v_{ta}\tau_{aa}}{n_{a}v_{ta}^{2}} \int_{0}^{\infty} dv v^{3} f_{a0}(x) \varphi_{m}(x) \nu_{D}^{ab}(v) \varphi_{m'}(x)
= \frac{\tau_{aa}}{n_{a}v_{ta}} \int_{0}^{\infty} dv v^{3} \frac{n_{a}}{\pi^{3/2}v_{ta}^{3}} e^{-x^{2}} \varphi_{m}(x) \frac{3\sqrt{\pi}}{4\tau_{ab}} \frac{[\phi(y) - G(y)]}{x^{3}} \varphi_{m'}(x)
= \frac{3}{4\pi} \frac{\tau_{aa}}{\tau_{ab}} \int_{0}^{\infty} dx e^{-x^{2}} \varphi_{m}(x) \varphi_{m'}(x) [\phi(y) - G(y)]
= \frac{3\sqrt{\pi}}{4\sqrt{h_{m}h_{m'}} \gamma} \frac{\tau_{aa}}{\tau_{ab}} \int_{0}^{\infty} dy e^{-(y^{2}/\gamma^{2})} L_{m}^{(3/2)}(y^{2}/\gamma^{2})
\times L_{m'}^{(3/2)}(y^{2}/\gamma^{2}) [\phi(y) - G(y)]. \quad (5.24)$$

The integral in the last equation may be evaluated upon substituting the definition for the associated Laguerre polynomials [29],

$$L_n^{(\alpha)}(x) = \sum_{k=0}^n \frac{(-1)^k}{k!} \binom{n+\alpha}{n-k} x^k,$$
 (5.25)

where the binomial coefficients are calculated from

$$\binom{p}{q} = \frac{p!}{q!(p-q)!} = \frac{\Gamma(p+1)}{\Gamma(q+1)\Gamma(p-q+1)}.$$
 (5.26)

This leads to the following expression,

$$\nu_{mm'}^{ab} = \sqrt{\pi} \frac{\tau_{aa}}{\tau_{ab}} \sum_{k=0}^{m} \sum_{k'=0}^{m'} \frac{S_{mm'}^{(k,k')}}{\gamma^{2(k+k')+1}} \int_{0}^{\infty} dy e^{-(y^2/\gamma^2)} y^{2(k+k')} [\phi(y) - G(y)], \quad (5.27)$$

with

$$S_{mm'}^{(k,k')} = \frac{3}{2} \left[\frac{\Gamma(m+1)\Gamma(m'+1)}{\Gamma(m+5/2)\Gamma(m'+5/2)} \right]^{1/2} \times \frac{(-1)^{k+k'}}{k! \ k'!} {m+3/2 \choose m-k} {m'+3/2 \choose m'-k'}.$$
 (5.28)

Using the relation

$$\phi(y) = \frac{2y}{\sqrt{\pi}} e^{-y^2} M(1, 3/2, y^2), \tag{5.29}$$

with M(a, b, z) being the confluent hypergeometric (or Kummer's) function (see, e.g., References 29 and 47), and the integral

$$\int_{0}^{\infty} dt e^{-st} t^{b-1} M(a, c, kt) = \frac{\Gamma(b)}{s^b} F(a, b; c; \frac{k}{s}), \quad |s| > |k|,$$
 (5.30)

where F(a, b; c; z) denotes the Gauss hypergeometric function [29, 47], one obtains for the integral involving the error function ϕ in Eq. (5.24)

$$\sqrt{\pi} \int_{0}^{\infty} dy e^{-(y^{2}/\gamma^{2})} y^{2(k+k')} \phi(y)$$

$$= \int_{0}^{\infty} dy e^{-(y^{2}/\gamma^{2})} y^{2(k+k')} 2y e^{-y^{2}} M(1, 3/2, y^{2})$$

$$= \int_{0}^{\infty} dt e^{-t(1+\gamma^{2})/\gamma^{2}} t^{k+k'} M(1, 3/2, t)$$

$$= \frac{\Gamma(k+k'+1)\gamma^{2(k+k'+1)}}{(1+\gamma^{2})^{k+k'+1}} F(1, k+k'+1; \frac{3}{2}; \frac{\gamma^{2}}{1+\gamma^{2}}). \quad (5.31)$$

Applying an integration by parts the integral involving the Chandrasekhar function G can be reduced to Eq. (5.31). It follows that

$$\sqrt{\pi} \int_{0}^{\infty} dy e^{-(y^{2}/\gamma^{2})} y^{2(k+k')} G(y)$$

$$= \sqrt{\pi} \int_{0}^{\infty} dy e^{-(y^{2}/\gamma^{2})} y^{2(k+k')} \left[\frac{(k+k')}{y^{2}} - \frac{1}{\gamma^{2}} \right] \phi(y)$$

$$= \int_{0}^{\infty} dy e^{-(y^{2}/\gamma^{2})} y^{2(k+k')} \left[\frac{(k+k')}{y^{2}} - \frac{1}{\gamma^{2}} \right] 2y e^{-y^{2}} M(1, 3/2, y^{2})$$

$$= \int_{0}^{\infty} dt e^{-t(1+\gamma^{2})/\gamma^{2}} \left[(k+k')t^{k+k'-1} - \frac{t^{k+k'}}{\gamma^{2}} \right] M(1, 3/2, t)$$

$$= \frac{\Gamma(k+k'+1)\gamma^{2(k+k')}}{(1+\gamma^{2})^{k+k'}}$$

$$\times \left[F(1, k+k'; \frac{3}{2}; \frac{\gamma^{2}}{1+\gamma^{2}}) - \frac{1}{(1+\gamma^{2})} F(1, k+k'+1; \frac{3}{2}; \frac{\gamma^{2}}{1+\gamma^{2}}) \right], (5.32)$$

where

$$\int dy G(y) = -\frac{\phi(y)}{2y} \tag{5.33}$$

has been used. Now, from Eq. (5.27) together with Eqs. (5.31) and (5.32), one obtains the individual species version of the matrix elements with respect to the Lorentz operator,

$$\nu_{mm'}^{ab}(\gamma_{ab}) = \frac{\tau_{aa}}{\tau_{ab}} \hat{\nu}_{mm'}^{ab}(\gamma_{ab}), \tag{5.34}$$

where $\hat{\nu}_{mm'}^{ab}$ is given by

$$\hat{\nu}_{mm'}^{ab}(\gamma_{ab}) = \sum_{k=0}^{m} \sum_{k'=0}^{m'} S_{mm'}^{(k,k')} P_{\nu}^{(k,k')}(\gamma_{ab}), \tag{5.35}$$

and with

$$P_{\nu}^{(k,k')}(\gamma) \equiv \frac{\Gamma(k+k'+1)}{\gamma(1+\gamma^2)^{k+k'}} \times \left[F(1,k+k'+1;\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) - F(1,k+k';\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) \right]. (5.36)$$

The quantity $S_{mm'}^{(k,k')}$ is given by Eq. (5.28) and the ratio of collision times is expressed as [22]

$$\frac{\tau_{aa}}{\tau_{ab}} = \frac{\hat{\nu}_{ab}}{\hat{\nu}_{aa}} = \frac{n_b e_b^2}{n_a e_a^2}.$$
 (5.37)

One can easily show that the double sum in Eq. (5.35) can be converted to a single sum giving the result

$$\hat{\nu}_{mm'}^{ab}(\gamma_{ab}) = \sum_{j=0}^{m+m'} X_{mm'}^{(j)} p_{\nu}^{(j)}(\gamma_{ab}), \qquad (5.38)$$

where

$$X_{mm'}^{(j)} = \sum_{k=0}^{j} S_{mm'}^{(k,j-k)}, \tag{5.39}$$

and

$$p_{\nu}^{(j)}(\gamma) \equiv \frac{j!}{\gamma(1+\gamma^2)^j} \left[F(1,j+1;\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) - F(1,j;\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) \right]. \tag{5.40}$$

Note that $S_{mm'}^{(k,k')}=0$ for k>m or k'>m'. Due to the fact that $X_{mm'}^{(j)}=X_{m'm}^{(j)}$ it immediately follows from Eq. (5.38) that the matrix elements are symmetric, that is $\nu_{mm'}^{ab}=\nu_{m'm}^{ab}$ [this could have also been seen directly from Eq. (5.24)].

Finally, the matrix elements of the 'full' Lorentz part of the collision operator are given by

$$\nu_{mm'}^{a} = \sum_{b} \nu_{mm'}^{ab}
= \nu_{mm'}^{aa} + \sum_{b \neq a} \nu_{mm'}^{ab}.$$
(5.41)

In a plasma where several different ion species are present the treatment of electron-ion collisions is simplified if one assumes the ions to be immobile [22]. That is to say, when infinitely heavy background ions are assumed, Eq. (5.40) is given by

$$p_{\nu}^{(j)}(z) = \frac{\sqrt{\pi}}{2} \Gamma(j+1/2) - \mathcal{O}(z^{j+1/2}), \tag{5.42}$$

where $z \equiv 1/(1 + \gamma_{ab}^2)$ tends to zero (for equal species temperatures the parameter z approximately corresponds to the ratio of particle masses m_a/m_b). A detailed derivation of the corresponding asymptotic expansion of $p_{\nu}^{(j)}$ will be given in Chapter 5.5. Using, e.g. MAPLE [48], the summation in Eq. (5.38) can now be performed to give the following 'closed' form of the matrix elements

$$\nu_{mm'}^{ab} = \frac{\tau_{aa}}{\tau_{ab}} \hat{\nu}_{mm'}^{a\infty} - \mathcal{O}(z^{1/2}) , \qquad (5.43)$$

with

$$\hat{\nu}_{mm'}^{a\infty} = \frac{\sqrt{\pi}}{5} \left[\frac{m!\Gamma(m'+5/2)}{m'!\Gamma(m+5/2)} \right]^{1/2} \left[5(m+1) - m' \right], \quad m \ge m' - 1. \quad (5.44)$$

From Eq. (5.41) one obtains for the electron version of the matrix elements regarding the pitch-angle scattering operator $\hat{\mathcal{L}} \equiv \mathcal{L}/|\lambda|$, [see Eq. (3.26) in Chapter 3]

$$\nu_{mm'}^e = \hat{\nu}_{mm'}^{ee} + Z_{\text{eff}} \hat{\nu}_{mm'}^{e\infty} \tag{5.45}$$

with the effective charge

$$Z_{\text{eff}} \equiv \frac{1}{n_e} \sum_{s} n_s Z_s^2, \tag{5.46}$$

where the sum is taken over all ion species.

5.2.2 Energy scattering part of $C_{ab}[f_{a1}, f_{b0}]$

By carrying out the same operations as for the calculation of the Lorentz operator matrix elements one arrives at the expression

$$\frac{1}{n_{a}v_{ta}^{2}} \int_{0}^{\infty} dv v^{3} \varphi_{m} \sum_{m'=0}^{M} \sum_{b} C_{ab}^{D,v} \left[f_{a0} f_{m'}^{\sigma,(k)} \varphi_{m'} \right]
= \sum_{m'=0}^{M} \sum_{b} \left(\frac{1}{n_{a}v_{ta}^{2}} \int_{0}^{\infty} dv v^{3} \varphi_{m} C_{ab}^{D,v} \left[f_{a0} \varphi_{m'} \right] \right) f_{m'}^{\sigma,(k)}
= \kappa \sum_{m'=0}^{M} \sum_{b} D_{mm'}^{ab} f_{m'}^{\sigma,(k)}(\lambda),$$
(5.47)

where the quantities $D_{mm'}^{ab}$ are the matrix elements of the energy scattering part of the collision operator defined by

$$D_{mm'}^{ab} \equiv v_{ta} \tau_{aa} \left(\varphi_m \left| v^{-1} \mathcal{C}_{ab}^{D,v} \right| \varphi_{m'} \right). \tag{5.48}$$

Recalling the definition of $C_{ab}^{D,v}$, Eq. (5.17), the expression for the associated matrix elements reads

$$D_{mm'}^{ab} = \frac{v_{ta}\tau_{aa}}{n_a v_{ta}^2} \int_0^\infty dv v^3 \varphi_m \mathcal{C}_{ab}^{D,v} [f_{a0}\varphi_{m'}]$$

$$= \frac{\tau_{aa}}{n_a v_{ta}} \int_0^\infty dv v \varphi_m \frac{\partial}{\partial v} \left[v^3 \left(\frac{m_a}{m_a + m_b} \nu_s^{ab} + \frac{1}{2} \nu_{\parallel}^{ab} v \frac{\partial}{\partial v} \right) \right] f_{a0}\varphi_{m'}. (5.49)$$

Substituting the definitions of the slowing down and parallel velocity diffusion frequency, respectively, into Eq. (5.49) and after performing the derivative with respect to normalized velocity in the second part of the equation one gets

$$D_{mm'}^{ab} = \frac{3}{4\pi} \frac{\tau_{aa}}{\tau_{ab}} \int_{0}^{\infty} \mathrm{d}x x \varphi_{m} \frac{\partial}{\partial x} \left[G(y) e^{-x^{2}} x \frac{\partial \varphi_{m'}}{\partial x} \right]$$

$$-2\left(1 - \frac{T_a}{T_b}\right)G(y)x^2e^{-x^2}\varphi_{m'}\right],$$
 (5.50)

where $\partial f_{a0}/\partial x = -2xf_{a0}$ has been used. Provided that $T_a = T_b = T$ and by means of Eq. (5.3) the last formula yields

$$D_{mm'}^{ab} = \frac{3\sqrt{\pi}\tau_{aa}}{4\sqrt{h_m h_{m'}}\tau_{ab}} \int_{0}^{\infty} \mathrm{d}x x L_m^{(3/2)}(x^2) \frac{\partial}{\partial x} \left[G(y) x e^{-x^2} \frac{\partial}{\partial x} L_{m'}^{(3/2)}(x^2) \right], \quad (5.51)$$

from which, by using Eq. (5.25), one obtains,

$$D_{mm'}^{ab} = \frac{3\sqrt{\pi}\tau_{aa}}{4\sqrt{h_{m}h_{m'}}\tau_{ab}} \sum_{k=0}^{m} \frac{(-1)^{k}}{k!} {m+3/2 \choose m-k} \times \int_{0}^{\infty} dx x^{2k+1} \frac{\partial}{\partial x} \left[G(y) x e^{-x^{2}} \frac{\partial}{\partial x} L_{m'}^{(3/2)}(x^{2}) \right].$$
 (5.52)

Here, Eq. (5.52) is readily evaluated applying again Eq. (5.25) as well as Eq. (5.32) along with an integration by parts. Thus, the individual species version of the matrix elements pertaining to the energy scattering part of $C_{ab}[f_{a1}, f_{b0}]$ is given as follows

$$D_{mm'}^{ab}(\gamma_{ab}) = -\sqrt{\pi} \frac{\tau_{aa}}{\tau_{ab}} \sum_{k=0}^{m} \sum_{k'=0}^{m'} S_{mm'}^{(k,k')}(2k+1)2k' \int_{0}^{\infty} dx e^{-x^{2}} x^{2(k+k')} G(y)$$

$$\equiv \frac{\tau_{aa}}{\tau_{ab}} \hat{D}_{mm'}^{ab}(\gamma_{ab}), \qquad (5.53)$$

with

$$\hat{D}_{mm'}^{ab}(\gamma_{ab}) = \sum_{k=0}^{m} \sum_{k'=0}^{m'} S_{mm'}^{(k,k')} P_D^{(k,k')}(\gamma_{ab}), \tag{5.54}$$

and where the ratio of collision times has been defined in Eq. (5.37). The quantity $P_D^{(k,k')}$ reads

$$P_D^{(k,k')}(\gamma) = \frac{2k'(2k+1)(k+k')!}{\gamma(1+\gamma^2)^{k+k'}} \times \left[\frac{1}{(1+\gamma^2)} F(1,k+k'+1;\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) - F(1,k+k';\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) \right]. (5.55)$$

Note that the matrix elements $\hat{D}_{m0}^{ab} \equiv 0$ following immediately from Eq. (5.51). Represented in terms of a single sum Eq. (5.54) can be rewritten

as

$$\hat{D}_{mm'}^{ab}(\gamma_{ab}) = \sum_{j=0}^{m+m'} Y_{mm'}^{(j)} p_D^{(j)}(\gamma_{ab}), \qquad (5.56)$$

where

$$Y_{mm'}^{(j)} = 2\sum_{k=0}^{j} S_{mm'}^{(k,j-k)}(2k+1)(j-k),$$
(5.57)

with $S_{mm'}^{(k,k')}$ introduced in Eq. (5.28) as well as

$$p_D^{(j)}(\gamma) = \frac{j!}{\gamma(1+\gamma^2)^j} \left[\frac{1}{(1+\gamma^2)} F(1,j+1;\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) - F(1,j;\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) \right]. \quad (5.58)$$

Similar to the pitch-angle scattering case the full version of the matrix elements is given through the sum of all contributions from collisions with particles of species b, that is

$$D_{mm'}^{a} = D_{mm'}^{aa} + \sum_{b \neq a} D_{mm'}^{ab}.$$
 (5.59)

Due to the fact that $D_{mm'}^{ab}$ is of $\mathcal{O}(z)$ (for details see again Chapter 5.5), where z tends to zero for the case when immobile background ions are assumed, it is feasible to neglect the contributions from background particles. Thus, because of $\hat{D}_{mm'}^{ee} \gg \hat{D}_{mm'}^{ei}$, one obtains from Eq. (5.59) for the electron version of the matrix elements,

$$D_{mm'}^e \approx \hat{D}_{mm'}^{ee}. (5.60)$$

5.3 Integral part of the collision operator

In this section the evaluation of collision matrix elements of the field particle part of the Coulomb operator (see, e.g., Reference 22 or Appendix B.4.2) is shown. This operator is responsible for momentum conservation and can be expressed as

$$\mathcal{C}_{ab}^{\mathcal{I}}[f_{b1}] \equiv \mathcal{C}_{ab}[f_{a0}, f_{b1}]
= L^{ab}f_{a0}\left[\frac{m_a}{m_b}f_{b1} + \frac{2}{v_{ta}^2}\varphi_{b1} + \left(1 - \frac{m_a}{m_b}\right)\frac{2v}{v_{ta}^2}\frac{\partial\varphi_{b1}}{\partial v} - \frac{4v^2}{v_{ta}^4}\frac{\partial^2\psi_{b1}}{\partial v^2}\right]
= \frac{3n_a e^{-x^2}}{\tau_{ab}n_b}\left[\frac{m_a}{m_b}f_{b1} + \frac{2}{v_{ta}^2}\varphi_{b1} + \frac{2y}{v_{ta}^2}\left(1 - \frac{m_a}{m_b}\right)\frac{\partial\varphi_{b1}}{\partial y} - \frac{4y^2}{v_{ta}^4}\frac{\partial^2\psi_{b1}}{\partial y^2}\right], (5.61)$$

with f_{b1} being the unknown field particle distribution function approximated by the expansion

$$f_{b1}(\lambda, y) \approx f_{b0}(y) \sum_{m'=0}^{M} f_{m'}^{\sigma,(k)}(\lambda) \varphi_{m'}(y)$$

$$\equiv f_{b0}(y) \sum_{m'=0}^{M} \hat{f}_{b,m'}(\lambda, y), \qquad (5.62)$$

and where the test functions $\varphi_{m'}$ have been defined in Eq. (5.3). Here, $f_{b0}(y) = n_b e^{-y^2}/(\pi^{3/2}v_{tb}^3)$ is the background Maxwellian and $y = v/v_{tb}$ is the normalized speed. The functionals φ_{b1} and ψ_{b1} , respectively, denote the Trubnikov potentials (see Appendix C).

5.3.1 φ -basis

The matrix elements of the field particle operator in terms of φ_m -basis are obtained from Eq. (5.61) acting on Eq. (5.62) followed by a multiplication on the left by $\varphi_m(x)$ along with an integration over $1/(n_a v_{ta}^2) \int_0^\infty dv v^3$. This leads to

$$\frac{1}{n_a v_{ta}^2} \int_0^\infty dv v^3 \varphi_m \sum_{m'=0}^M \sum_b \mathcal{C}_{ab}^{\mathcal{I}} \left[f_{b0} f_{m'}^{\sigma,(k)} \varphi_{m'} \right]$$

$$= \kappa \sum_{m'=0}^M \sum_b \frac{v_{ta} \tau_{aa}}{n_a v_{ta}^2} \int_0^\infty dv v^3 \varphi_m \mathcal{C}_{ab}^{\mathcal{I}} \left[f_{b0} f_{m'}^{\sigma,(k)} \varphi_{m'} \right]$$

$$= \kappa \sum_{m'=0}^M \sum_b \mathcal{K}_{mm'}^{ab} \left[f_{m'}^{\sigma,(k)} \right], \qquad (5.63)$$

with $\mathcal{K}^{ab}_{mm'}$ representing an integral operator formally defined by

$$\mathcal{K}_{mm'}^{ab} \equiv v_{ta} \tau_{aa} \left(\varphi_m \left| v^{-1} \mathcal{C}_{ab}^{\mathcal{I}} \right| \varphi_{m'} \right). \tag{5.64}$$

From Eq. (5.61) it follows that the unknown distribution function f_{b1} , or more precisely the corresponding angular part $f_{m'}^{\sigma,(k)}$, appears under an integral (via the Trubnikov potentials, φ_{b1} and ψ_{b1} , respectively). Since these functionals are only known in terms of the so-called Burnett functions (see Chapter A and also Appendix C) it is convenient first to evaluate the desired matrix elements using these basis functions followed by a transformation to the φ_m -test functions.

In Chapter A the representation of an arbitrary function in terms of Burnett functions, $B_n^{(\ell)}(\lambda, z) = P_\ell(\lambda) p_n^{(\ell)}(z)$, has been derived. Applying the corresponding results to φ_m and $\hat{f}_{b,m'}$ one obtains

$$\varphi_m(x) = 2\sum_n \frac{B_n^{(0)}(x)}{h_n^{(0)}} \langle \varphi_m | p_n^{(0)} \rangle_v$$
 (5.65)

and

$$\hat{f}_{b,m'}(\lambda,y) \equiv f_{m'}^{\sigma,(k)}(\lambda)\varphi_{m'}(y)$$

$$= \sum_{\ell,n'} \frac{B_{n'}^{(\ell)}(\lambda,y)}{h_{n'}^{(\ell)}} \langle f_{m'}^{\sigma,(k)} | P_{\ell} \rangle_{\lambda'} \langle \varphi_{m'} | p_{n'}^{(\ell)} \rangle_{v'}, \qquad (5.66)$$

respectively. The radial scalar product between the test function φ_m and the function $p_n^{(\ell)}$ in Eqs. (5.65) as well as (5.66) corresponds to a transformation matrix which will be abbreviated by

$$\phi_{mn}^{(\ell)} = \phi_{nm}^{(\ell)} \equiv \langle \varphi_m | p_n^{(\ell)} \rangle, \tag{5.67}$$

where the quantity $p_n^{(\ell)}(x) \equiv x^{\ell} L_n^{(\ell+1/2)}(x^2)$. After substitution of Eqs. (5.65) and (5.66) into the relation for the integral operator $\mathcal{K}_{mm'}^{ab}$ it follows that

$$\mathcal{K}_{mm'}^{ab} \left[f_{m'}^{\sigma,(k)} \right] = \frac{\tau_{aa}}{n_a v_{ta}} \int_{0}^{\infty} dv v^3 2 \sum_{n} \frac{B_{n}^{(0)}(x)}{h_{n}^{(0)}} \phi_{mn}^{(0)} \\
\times \mathcal{C}_{ab}^{\mathcal{I}} \left[f_{b0}(y) \sum_{\ell,n'} \frac{B_{n'}^{(\ell)}(\lambda,y)}{h_{n'}^{(\ell)}} \langle f_{m'}^{\sigma,(k)} | P_{\ell} \rangle_{\lambda'} \phi_{m'n'}^{(\ell)} \right] \\
= \frac{\tau_{aa}}{\tau_{ab}} \frac{\tau_{ab}}{n_a v_{ta}} \sum_{n} \sum_{\ell,n'} \frac{2\phi_{mn}^{(0)}}{h_{n}^{(0)} h_{n'}^{(\ell)}} \int_{0}^{\infty} dv v^3 B_{n}^{(0)}(x) \\
\times \mathcal{C}_{ab}^{\mathcal{I}} \left[f_{b0}(y) B_{n'}^{(\ell)}(\lambda,y) \right] \phi_{n'm'}^{(\ell)} \langle f_{m'}^{\sigma,(k)} | P_{\ell} \rangle_{\lambda'} \\
\equiv \frac{\tau_{aa}}{\tau_{ab}} \hat{\mathcal{K}}_{mm'}^{ab} \left[f_{m'}^{\sigma,(k)} \right], \qquad (5.68)$$

with

$$\hat{\mathcal{K}}_{mm'}^{ab} \left[f_{m'}^{\sigma,(k)} \right] = \sum_{\ell} P_{\ell}(\lambda) \sum_{n,n'} \frac{2\phi_{mn}^{(0)}}{h_n^{(0)} h_{n'}^{(\ell)}} \hat{I}_{nn'}^{(\ell)} \phi_{n'm'}^{(\ell)} \langle f_{m'}^{\sigma,(k)} | P_{\ell} \rangle_{\lambda'}, \tag{5.69}$$

and where the quantity

$$\hat{I}_{nn'}^{(\ell)}(\gamma_{ab}) = \frac{\tau_{ab}}{v_{ta}} \langle p_n^{(0)} | v \mathcal{C}_{ab}^{\mathcal{I}} | p_{n'}^{(\ell)} \rangle_v
= \frac{\tau_{ab}}{n_a v_{ta}} \int_0^\infty dv v^3 p_n^{(0)}(x) \mathcal{C}_{ab}^{\mathcal{I}} \left[f_{b0}(y) p_{n'}^{(\ell)}(y) \right]$$
(5.70)

denotes the radial part of the matrix elements of the field particle operator in terms of Burnett functions. From Eq. (5.69) one can infer that the matrix elements in the φ_m -basis are given through

$$I_{mm'}^{(\ell)}(\gamma_{ab}) = \sum_{n=0}^{N} \sum_{n'=0}^{N'} \frac{2}{h_n^{(0)} h_{n'}^{(\ell)}} \phi_{mn}^{(0)} \hat{I}_{nn'}^{(\ell)} \phi_{n'm'}^{(\ell)}, \tag{5.71}$$

where $h_n^{(\ell)} = \Gamma(n+\ell+3/2)/[2\pi^{3/2}n!(\ell+1/2)]$. The values for N and N' have to be chosen as large as possible in order to achieve accurate numerical results for $I_{mm'}^{(\ell)}$. In Chapter 5.4 it will be shown that the sum over n can be truncated at n=m which, of course, is a considerable numerical advantage gained by the fact that $M \ll N$ (roughly speaking, the order of magnitude of M and N is 10 and 10⁶, respectively). Upon defining the quantity

$$K_{mm'}^{ab}(\lambda, \lambda') = \sum_{\ell=0}^{L} P_{\ell}(\lambda) P_{\ell}(\lambda') I_{mm'}^{(\ell)}, \qquad (5.72)$$

the individual species version of the integral operator $\hat{K}^{ab}_{mm'}$ can be represented as an angular scalar product between $K^{ab}_{mm'}$ and the unknown function $f^{\sigma,(k)}_{m'}$, that is,

$$\hat{K}_{mm'}^{ab} \left[f_{m'}^{\sigma,(k)} \right] = \langle K_{mm'}^{ab}(\lambda, \lambda') | f_{m'}^{\sigma,(k)}(\lambda') \rangle_{\lambda'}$$

$$= \int_{-1}^{1} d\lambda' K_{mm'}^{ab}(\lambda, \lambda') f_{m'}^{\sigma,(k)}(\lambda'), \qquad (5.73)$$

whereas the full version follows from

$$\mathcal{K}_{mm'}^{a} = \mathcal{K}_{mm'}^{aa} + \sum_{b \neq a} \mathcal{K}_{mm'}^{ab}.$$
 (5.74)

In Chapter 5.5.2 it will be shown in detail that the second part on the RHS of Eq. (5.74) is at least of $\mathcal{O}(z^{1/2})$, where z tends to zero for infinitely heavy

background ions. Consequently, for the electron version of the matrix elements it is sufficient, due to $\hat{\mathcal{K}}^{ee}_{mm'} \gg \hat{\mathcal{K}}^{ei}_{mm'}$, to include only the term accounting for momentum conservation in electron electron collisions,

$$\mathcal{K}_{mm'}^e \approx \hat{\mathcal{K}}_{mm'}^{ee}.\tag{5.75}$$

Putting together the above results, that is to say Eqs. (5.6), (5.8), (5.22), (5.47) and (5.63), the drift kinetic equation, Eq. (5.1), is transformed to a set of coupled two dimensional differential equations for the coefficients $f_m^{\sigma,(k)}$ yielding

$$\sigma|\lambda| \frac{\partial f_{m}^{\sigma,(k)}}{\partial s} - \kappa \sum_{m'=0}^{M} \left\{ \nu_{mm'}^{e} \mathcal{L} \left[f_{m'}^{\sigma,(k)} \right] + D_{mm'}^{e} f_{m'}^{\sigma,(k)} + \mathcal{K}_{mm'}^{e} \left[f_{m'}^{\sigma,(k)} \right] \right\} = |\lambda| q_{k}^{\sigma} a_{m}^{(k)}, (5.76)$$

from which one obtains the desired Eq. (3.26) after dividing Eq. (5.76) by pitch-angle parameter $|\lambda|$. As mentioned above, the resulting equation is to be solved numerically in the code NEO-2 [31,46].

5.3.2 Burnett basis

The next quantity to be calculated is $\hat{I}_{nn'}^{(\ell)}(\gamma)$ [cf. Eq. (5.70)] representing the radial part of the matrix elements of the integral part of the collision operator in the Burnett function basis. The field particle operator can be written as

$$C_{ab}^{\mathcal{I}}\left[f_{b0}p_{n'}^{(\ell)}\right] = \frac{3n_{a}e^{-x^{2}}}{\tau_{ab}n_{b}}\left[\frac{m_{a}}{m_{b}}f_{b0}p_{n'}^{(\ell)} + \frac{2}{v_{ta}^{2}}\varphi_{b1,y} + \frac{2y}{v_{ta}^{2}}\left(1 - \frac{m_{a}}{m_{b}}\right)\frac{\partial\varphi_{b1,y}}{\partial y} - \frac{4y^{2}}{v_{ta}^{4}}\frac{\partial^{2}\psi_{b1,y}}{\partial y^{2}}\right], \quad (5.77)$$

where

$$f_{b0}p_{n'}^{(\ell)} = \frac{n_b}{\pi^{3/2}v_{tb}^3}e^{-y^2}y^{\ell}L_{n'}^{(\ell+1/2)}(y^2), \tag{5.78}$$

and the radial part of the Trubnikov potentials is given as

$$\varphi_{b1,y} = -\frac{n_b}{2\pi^{3/2}v_{tb}}\hat{\varphi}_{n'}^{(\ell)}(y)$$
 (5.79)

$$\psi_{b1,y} = -\frac{n_b v_{tb}}{4\pi^{3/2}} \hat{\psi}_{n'}^{(\ell)}(y). \tag{5.80}$$

The evaluation of these functionals will be shown explicitly in Appendices C.1 and C.2. The corresponding results for $\hat{\varphi}_{n'}^{(\ell)}$ and $\hat{\psi}_{n'}^{(\ell)}$ are

$$\hat{\varphi}_0^{(\ell)} = \frac{\gamma(\ell+1/2, y^2)}{2y^{\ell+1}} \tag{5.81}$$

$$\hat{\varphi}_{n'}^{(\ell)} = \frac{1}{2n'} e^{-y^2} y^{\ell} L_{n'-1}^{(\ell+1/2)}(y^2), \quad \text{for} \quad n' \ge 1$$
 (5.82)

$$\hat{\psi}_0^{(\ell)} = \frac{1}{2} \left[\hat{\varphi}_0^{(\ell)} - y \hat{\varphi}_0^{(\ell-1)} \right]$$
 (5.83)

$$\hat{\psi}_{n'}^{(\ell)} = -\frac{1}{2n'} \hat{\varphi}_{n'-1}^{(\ell)}, \quad \text{for} \quad n' \ge 1.$$
 (5.84)

By means of Eq. (5.82), Eq. (5.78) may be expressed in terms of the function $\hat{\varphi}_{n'}^{(\ell)}$. It follows that

$$f_{b0}p_{n'}^{(\ell)} = \frac{n_b}{\pi^{3/2}v_{tb}^3} 2(n'+1)\hat{\varphi}_{n'+1}^{(\ell)}(y), \quad \text{for} \quad n' \ge 0.$$
 (5.85)

The first derivative of $\hat{\varphi}_{n'}^{(\ell)}$ as well as the second derivative of $\hat{\psi}_{n'}^{(\ell)}$, respectively, with respect to normalized speed become (see again Appendices C.1 and C.2)

$$y \frac{\partial \hat{\varphi}_{n'}^{(\ell)}}{\partial y} = 2(n'+1)\hat{\varphi}_{n'+1}^{(\ell)} - (2n'+\ell+1)\hat{\varphi}_{n'}^{(\ell)}$$
 (5.86)

$$y^{2} \frac{\partial^{2} \hat{\psi}_{0}^{(\ell)}}{\partial y^{2}} = \frac{(\ell+1)(\ell+2)}{2} \hat{\varphi}_{0}^{(\ell)} - \frac{\ell(\ell-1)}{2} y \hat{\varphi}_{0}^{(\ell-1)} - 2\hat{\varphi}_{1}^{(\ell)}$$
 (5.87)

$$y^{2} \frac{\partial^{2} \hat{\varphi}_{n'-1}^{(\ell)}}{\partial y^{2}} = 4n'(n'+1)\hat{\varphi}_{n'+1}^{(\ell)} - 2n'(4n'+2\ell+1)\hat{\varphi}_{n'}^{(\ell)} + (2n'+\ell)(2n'+\ell-1)\hat{\varphi}_{n'-1}^{(\ell)}.$$

$$(5.88)$$

Summing up the above results Eq. (5.77) can be expressed in terms of the function $\hat{\varphi}_{n'}^{(\ell)}$. For $n' \geq 2$ one obtains

$$\mathcal{C}_{ab}^{\mathcal{I}}\left[f_{b0}p_{n'}^{(\ell)}\right] = -\frac{3n_{a}e^{-x^{2}}}{\pi^{3/2}\tau_{ab}v_{tb}^{3}\gamma^{4}} \left\{ (2n'+\ell)\frac{(2n'+\ell-1)}{2n'}\hat{\varphi}_{n'-1}^{(\ell)} - \left[(2n'+\ell+1)\left(1-\frac{T_{a}}{T_{b}}\right) + (2n'+\ell)(1+\gamma^{2})\right]\hat{\varphi}_{n'}^{(\ell)} + 2(n'+1)(1+\gamma^{2})\left(1-\frac{T_{a}}{T_{b}}\right)\hat{\varphi}_{n'+1}^{(\ell)} \right\}.$$
(5.89)

Assuming equal species temperatures, $T_a = T_b = T$, it follows from the last equation that

$$\mathcal{C}_{ab}^{\mathcal{I}} \left[f_{b0} p_{n'}^{(\ell)} \right] = \frac{3n_a e^{-x^2}}{\pi^{3/2} \tau_{ab} v_{tb}^3} \frac{(2n' + \ell)}{\gamma^4} \times \left[(1 + \gamma^2) \hat{\varphi}_{n'}^{(\ell)} - \frac{(2n' + \ell - 1)}{2n'} \hat{\varphi}_{n'-1}^{(\ell)} \right].$$
(5.90)

The matrix elements of the field particle part of the collision operator in the Burnett basis are calculated from

$$\hat{I}_{nn'}^{(\ell)}(\gamma) = \frac{\tau_{ab}}{n_a v_{ta}} \int_0^\infty dv v^3 p_n^{(0)}(x) \mathcal{C}_{ab}^{\mathcal{I}} \left[f_{b0}(y) p_{n'}^{(\ell)}(y) \right]
= \frac{3(2n'+\ell)}{\pi^{3/2} \gamma^5} \int_0^\infty dy y^3 L_n^{(1/2)}(y^2/\gamma^2) e^{-y^2/\gamma^2}
\times \left[(1+\gamma^2) \hat{\varphi}_{n'}^{(\ell)}(y) - \frac{(2n'+\ell-1)}{2n'} \hat{\varphi}_{n'-1}^{(\ell)}(y) \right]
= \frac{3(2n'+\ell)}{\pi^{3/2} \gamma^5} \left[(1+\gamma^2) U_{nn'}^{(\ell)} - \frac{(2n'+\ell-1)}{2n'} U_{nn'-1}^{(\ell)} \right], \quad (5.91)$$

for $n' \ge 2$. Here, $p_n^{(0)}(x) = L_n^{(1/2)}(x^2)$, $y = \gamma x$ and Eq. (5.90) has been applied and the auxiliary quantity

$$U_{n\eta}^{(\ell)}(\gamma) \equiv \int_{0}^{\infty} dy y^{3} L_{n}^{(1/2)}(y^{2}/\gamma^{2}) e^{-y^{2}/\gamma^{2}} \hat{\varphi}_{\eta}^{(\ell)}(y)$$
 (5.92)

has been introduced. After substituting into this equation the definition of the associated Laguerre polynomials [29]

$$L_n^{(1/2)}(y^2/\gamma^2) = \sum_{k=0}^n \frac{(-1)^k}{k!\gamma^{2k}} \binom{n+1/2}{n-k} y^{2k}, \tag{5.93}$$

as well as

$$\hat{\varphi}_{\eta}^{(\ell)} = \frac{1}{2\eta} e^{-y^2} y^{\ell} L_{\eta-1}^{(\ell+1/2)}(y^2), \tag{5.94}$$

it follows that Eq. (5.92) may be rewritten in the form

$$U_{n\eta}^{(\ell)} = \frac{1}{2\eta} \sum_{k=0}^{n} \frac{(-1)^k}{k! \gamma^{2k}} {n+1/2 \choose n-k} V_{\eta}^{(\ell)}(k,\gamma),$$
 (5.95)

with

$$V_{\eta}^{(\ell)}(k,\gamma) \equiv \int_{0}^{\infty} dy e^{-y^{2}(1+\gamma^{-2})} y^{\ell+2k+3} L_{\eta-1}^{(\ell+1/2)}(y^{2}).$$
 (5.96)

The solution of this integral can be obtained with the help of Reference 29 where one finds

$$\int_{0}^{\infty} dt e^{-st^{2}} t^{2\beta+1} L_{n}^{\alpha}(t^{2}) = \frac{\Gamma(\beta+1)\Gamma(\alpha+n+1)}{2\Gamma(n+1)\Gamma(\alpha+1)s^{\beta+1}} F(-n,\beta+1;\alpha+1;\frac{1}{s}), (5.97)$$

valid for Re $\beta > -1$ and Re s > 0, and where F(a, b; c; z) again denotes the Gauss hypergeometric function. Thus, Eq. (5.96) has the result

$$V_{\eta}^{(\ell)}(k,\gamma) = \frac{\Gamma(\ell/2 + k + 2)\Gamma(\eta + \ell + 1/2)\gamma^{\ell+2k+4}}{2\Gamma(\eta)\Gamma(\ell + 3/2)(1 + \gamma^2)^{\ell/2+k+2}} \times F(1 - \eta, \frac{\ell}{2} + k + 2; \ell + \frac{3}{2}; \frac{\gamma^2}{1+\gamma^2}), \tag{5.98}$$

which can be utilized in Eq. (5.95) yielding

$$U_{n\eta}^{(\ell)} = \frac{\Gamma(\eta + \ell + 1/2)\gamma^{\ell+4}}{4\Gamma(\eta + 1)\Gamma(\ell + 3/2)(1 + \gamma^2)^{\ell/2+2}} \sum_{k=0}^{n} \frac{(-1)^k}{k!} {n+1/2 \choose n-k} \times \frac{\Gamma(\ell/2 + k + 2)}{(1 + \gamma^2)^k} F(1 - \eta, \frac{\ell}{2} + k + 2; \ell + \frac{3}{2}; \frac{\gamma^2}{1+\gamma^2}).$$
 (5.99)

In case that $\ell = 0$ one can find a simpler relation instead of cumbersome Eq. (5.99), that is to say

$$U_{n\eta}^{(0)} = \frac{\pi}{8} \gamma^3 \delta_{0n+\eta} - \frac{\gamma^4}{6(1+\gamma^2)^2} {\eta-5/2 \choose \eta} \times {n+1/2 \choose n} F(1-n-\eta, 2; \frac{5}{2} - \eta; \frac{1}{1+\gamma^2}),$$
 (5.100)

which has been computed by means of MAPLE [48].

Recalling Eq. (5.91) and taking into account Eq. (5.99) one finally arrives at the following expression for the matrix elements of the field particle operator in terms of Burnett functions,

$$\hat{I}_{nn'}^{(\ell)}(\gamma_{ab}) = \frac{3}{4\pi^{3/2}} \frac{(2n'+\ell)\Gamma(n'+\ell+1/2)}{\Gamma(n'+1)\Gamma(\ell+3/2)} \frac{\gamma_{ab}^{\ell-1}}{(1+\gamma_{ab}^2)^{\ell/2+1}}$$

$$\times \sum_{k=0}^{n} \frac{(-1)^{k}}{k!} \binom{n+1/2}{n-k} \frac{\Gamma(\ell/2+k+2)}{(1+\gamma_{ab}^{2})^{k}} \mathcal{P}_{n'}^{(\ell)}(k,\gamma_{ab}) (5.101)$$

$$= \frac{h_{n}^{(0)} h_{n'}^{(\ell)}}{2} \frac{6\pi^{3/2} (2n'+\ell)n!}{(2n'+2\ell+1)\Gamma(\ell+1/2)} \frac{\gamma_{ab}^{\ell-1}}{(1+\gamma_{ab}^{2})^{\ell/2+1}}$$

$$\times \sum_{k=0}^{n} \frac{(-1)^{k}}{k!} \frac{\Gamma(\ell/2+k+2)}{(n-k)!\Gamma(k+3/2)} \frac{\mathcal{P}_{n'}^{(\ell)}(k,\gamma_{ab})}{(1+\gamma_{ab}^{2})^{k}}, (5.102)$$

valid for $n' \geq 0$, and where

$$P_{n'}^{(\ell)}(k,\gamma) = F(1-n',\frac{\ell}{2}+k+2;\ell+\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) - \frac{(2n'+\ell-1)}{(2n'+2\ell-1)(1+\gamma^2)}F(2-n',\frac{\ell}{2}+k+2;\ell+\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}). (5.103)$$

The proof that Eq. (5.101) essentially includes n' = 0 and n' = 1 is not difficult but somewhat tedious [by using Eqs.(5.81)-(5.88), applying some properties of hypergeometric functions and again by means of MAPLE] and has been omitted here. Here it has to be mentioned that $\hat{I}_{n0}^{(0)} \equiv 0$, following directly from Eq. (5.101).

It turns out that for the case when the parameter ℓ is equal to one one can derive a much simpler expression for the matrix elements than that in Eq. (5.101). In virtue of Eq. (5.91) it follows that

$$\hat{I}_{nn'}^{(1)}(\gamma) = \frac{3(2n'+1)}{\pi^{3/2}\gamma^5} \left[(1+\gamma^2) \mathcal{U}_{nn'}^{(1)}(\gamma) - \mathcal{U}_{nn'-1}^{(1)}(\gamma) \right], \tag{5.104}$$

where

$$U_{n\eta}^{(1)} = \int_{0}^{\infty} dy y^{3} L_{n}^{(1/2)}(y^{2}/\gamma^{2}) e^{-y^{2}/\gamma^{2}} \hat{\varphi}_{\eta}^{(1)}(y)
= \frac{1}{2\eta} \int_{0}^{\infty} dy e^{-y^{2}(1+\gamma^{-2})} y^{4} L_{n}^{(1/2)}(y^{2}/\gamma^{2}) L_{\eta-1}^{(3/2)}(y^{2})
= \frac{1}{4\eta} \int_{0}^{\infty} dt e^{-t(1+\gamma^{-2})} t^{3/2} L_{n}^{(1/2)}(t/\gamma^{2}) L_{\eta-1}^{(3/2)}(t).$$
(5.105)

By using the following recurrence relation for the associated Laguerre polynomials [29] with respect to ℓ

$$L_n^{(1/2)}(x) = L_n^{(3/2)}(x) - L_{n-1}^{(3/2)}(x), (5.106)$$

as well as the integral

$$\int_{0}^{\infty} dt e^{-t(1+\gamma^{-2})} t^{\alpha} L_{N}^{(\alpha)}(t/\gamma^{2}) L_{M}^{(\alpha)}(t)$$

$$= \frac{\Gamma(M+N+\alpha+1)}{M!N!} \frac{\gamma^{2(N+\alpha+1)}}{(1+\gamma^{2})^{M+N+\alpha+1}}, \quad (5.107)$$

valid for Re $\alpha > -1$ and Re $(1 + \gamma^{-2}) > 0$ (which has been found in Reference 29) it follows from Eq. (5.105) that

$$U_{n\eta}^{(1)}(\gamma) = \frac{\Gamma(n+\eta+3/2)}{4n!\eta!} \frac{\gamma^{2n+5}}{(1+\gamma^2)^{n+\eta+3/2}} - \frac{n\Gamma(n+\eta+1/2)}{4n!\eta!} \frac{\gamma^{2n+3}}{(1+\gamma^2)^{n+\eta+1/2}}.$$
 (5.108)

Upon substituting this result into Eq. (5.104) and after rearranging terms one finds

$$\hat{I}_{nn'}^{(1)}(\gamma) = \frac{3(2n'+1)}{16\pi^{3/2}} \frac{\Gamma(n+n'-1/2)}{n!n'!} \frac{\gamma^{2n-2}}{(1+\gamma^2)^{n+n'+1/2}} \times \left[\gamma^2(4nn'+2n+2n'-1)-2n(2n-1)\right]. \quad (5.109)$$

This special case can be used as a first check for the numerical routine that computes Eq. (5.101).

5.4 Transformation matrix

The radial scalar product of the test functions φ_m and the radial part of the Burnett functions $p_n^{(\ell)}$ defines the transformation matrix between these two sets of orthonormal functions (see Appendix A.2),

$$\phi_{mn}^{(\ell)} = \phi_{nm}^{(\ell)} \equiv \langle \varphi_m | p_n^{(\ell)} \rangle_v. \tag{5.110}$$

Upon employing Eq. (A.22) it follows that

$$\phi_{mn}^{(\ell)} = \frac{1}{n_b} \int_0^\infty dv v^2 \frac{n_b e^{-y^2}}{\pi^{3/2} v_{tb}^3} \frac{\pi^{3/4}}{\sqrt{h_m}} L_m^{(3/2)}(y^2) y^\ell L_n^{(\ell+1/2)}(y^2)$$

$$= \frac{1}{\pi^{3/4} \sqrt{h_m}} \int_0^\infty dy e^{-y^2} y^{\ell+2} L_m^{(3/2)}(y^2) L_n^{(\ell+1/2)}(y^2)$$

$$= \frac{\Gamma_{mn}^{(\ell)}}{\pi^{3/4} \sqrt{h_m}}, \qquad (5.111)$$

where the integral in this equation has been given the abbreviated notation

$$T_{mn}^{(\ell)} \equiv \int_{0}^{\infty} dy e^{-y^{2}} y^{\ell+2} L_{m}^{(3/2)}(y^{2}) L_{n}^{(\ell+1/2)}(y^{2})$$

$$= \frac{1}{2} \int_{0}^{\infty} dt e^{-t} t^{(\ell+1)/2} L_{m}^{(3/2)}(t) L_{n}^{(\ell+1/2)}(t). \tag{5.112}$$

With the help of the orthogonality relation for the associated Laguerre polynomials

$$\int_{0}^{\infty} dt e^{-t} t^{\lambda} L_{m}^{(\lambda)}(t) L_{n}^{(\lambda)}(t) = \frac{\Gamma(n+\lambda+1)}{n!} \delta_{nm}, \quad \text{for } \text{Re } \lambda > -1, \quad (5.113)$$

and by using the following property with respect to finite summation [29],

$$L_m^{(\lambda+1)} = \sum_{k=0}^{m} L_k^{(\lambda)}, \tag{5.114}$$

it is straightforward to calculate the transformation matrix for ℓ is equal to zero. One has

$$T_{mn}^{(0)} = \frac{1}{2} \int_{0}^{\infty} dt e^{-t} t^{1/2} L_{m}^{(3/2)}(t) L_{n}^{(1/2)}(t)$$

$$= \sum_{k=0}^{m} \frac{1}{2} \int_{0}^{\infty} dt e^{-t} t^{1/2} L_{k}^{(1/2)}(t) L_{n}^{(1/2)}(t)$$

$$= \sum_{k=0}^{m} \frac{\Gamma(n+3/2)}{2n!} \delta_{nk}, \qquad (5.115)$$

from which one can infer that

$$T_{mn}^{(0)} = \begin{cases} \frac{\Gamma(n+3/2)}{2n!} & \text{for } n \le m \\ 0 & \text{for } n > m. \end{cases}$$
 (5.116)

An important detail concerning the numerical implementation of computation of the matrix elements $I_{mm'}^{(\ell)}$ is the fact that the transformation matrix $T_{mn}^{(0)}$ is equal to zero for n bigger than m. In that case, the sum over n in Eq. (5.71)

can be truncated at n = m, where the parameter m takes at most the value M which, in turn, is several orders of magnitude smaller than N. Thus, the computing time necessary for calculating the matrix elements is considerably reduced.

The evaluation of Eq. (5.112) for arbitrary ℓ can be performed by means of the relation (see Reference 29)

$$\int_{0}^{\infty} dt e^{-t} t^{\gamma - 1} L_n^{(\mu)}(t) = \frac{\Gamma(\gamma)\Gamma(n + \mu - \gamma + 1)}{n!\Gamma(\mu - \gamma + 1)}, \quad \text{for } \operatorname{Re} \gamma > 0. \quad (5.117)$$

By applying the definition [see Eq. (5.25)] of the associated Laguerre polynomials as well as Eq. (5.117) one obtains two solutions for $T_{mn}^{(\ell)}$ depending on which of the Laguerre polynomial is being replaced by Eq. (5.25), that is

$$T_{mn}^{(\ell)} = \frac{1}{2} \int_{0}^{\infty} dt e^{-t} t^{(\ell+1)/2} L_{m}^{(3/2)}(t) L_{n}^{(\ell+1/2)}(t)$$

$$= \sum_{k=0}^{n} \frac{(-1)^{k}}{2k!} {n+\ell+1/2 \choose n-k} \int_{0}^{\infty} dt e^{-t} t^{(\ell+1)/2+k} L_{m}^{(3/2)}(t)$$

$$= \sum_{k=0}^{n} \frac{(-1)^{k}}{k!} {n+\ell+1/2 \choose n-k} \frac{\Gamma(k+\ell/2+3/2)\Gamma(m+1-\ell/2-k)}{2m!\Gamma(1-\ell/2-k)}, (5.118)$$

and

$$T_{mn}^{(\ell)} = \frac{1}{2} \int_{0}^{\infty} dt e^{-t} t^{(\ell+1)/2} L_{m}^{(3/2)}(t) L_{n}^{(\ell+1/2)}(t)$$

$$= \sum_{k=0}^{m} \frac{(-1)^{k}}{2k!} {m+3/2 \choose m-k} \int_{0}^{\infty} dt e^{-t} t^{(\ell+1)/2+k} L_{n}^{(\ell+1/2)}(t)$$

$$= \sum_{k=0}^{m} \frac{(-1)^{k}}{k!} {m+3/2 \choose m-k} \frac{\Gamma(k+\ell/2+3/2)\Gamma(n+\ell/2-k)}{2n!\Gamma(\ell/2-k)}, \quad (5.119)$$

respectively, from which one obtains the transformation matrix $\phi_{mn}^{(\ell)}$ upon dividing the last two equations by the factor $\pi^{3/4}\sqrt{h_m}$. Carrying out the sum appearing in Eqs. (5.118) and (5.119) with MAPLE [48] yields the results

$$T_{mn}^{(\ell)} = \frac{\Gamma(\ell/2 + 3/2)\Gamma(m + 1 - \ell/2)}{2m!\Gamma(1 - \ell/2)} \times {\binom{n + \ell + 1/2}{n}}_{3}F_{2}(-n, \frac{\ell}{2}, \frac{\ell+3}{2}; \ell + \frac{3}{2}, \frac{\ell}{2} - m; 1), \qquad (5.120)$$

and

$$T_{mn}^{(\ell)} = \frac{\Gamma(\ell/2 + 3/2)\Gamma(n + \ell/2)}{2n!\Gamma(\ell/2)} \times {m + 3/2 \choose m} {}_{3}F_{2}(-m, 1 - \frac{\ell}{2}, \frac{\ell+3}{2}; \frac{5}{2}, 1 - n - \frac{\ell}{2}; 1), \qquad (5.121)$$

where $_3F_2$ indicates a generalized hypergeometric function [29]. These equations are unrestricted valid for odd values of ℓ , whereas for even $\ell > 0$ the elements of the transformation matrix are zero if $m > n + \ell/2 - 1$. Here, it has to be noted that in Eq. (5.120) the generalized hypergeometric function $_3F_2(a_1, a_2, a_3; b_1, b_2; 1)$ does not exist when an appropriate negative integer [like in Eq. (5.121)] is missing in the first list of parameters to compensate the negative integers (or zero) occurring in the second list for the case when $\ell/2 - m \leq 0$. This case is covered by the equation

$$T_{mn}^{(\ell)} = \sum_{k=m+1-\ell/2}^{n} \frac{(-1)^k}{k!} {n+\ell+1/2 \choose n-k} \frac{\Gamma(k+\ell/2+3/2)\Gamma(m+1-\ell/2-k)}{2m!\Gamma(1-\ell/2-k)}$$

$$= \frac{(-1)^{\ell/2+1}\Gamma(m+5/2)\Gamma(n+\ell+3/2)}{2\Gamma(m+2-\ell/2)\Gamma(n-m+\ell/2)\Gamma(m+\ell/2+5/2)}$$

$$\times {}_{3}F_{2}(m+1,m+\frac{5}{2},m+1-n-\frac{\ell}{2};m+2-\frac{\ell}{2},m+\frac{\ell}{2}+\frac{5}{2};1), \quad (5.122)$$

which has again been computed using MAPLE. Because of the fact that there exist various recurrence identities (see, e.g., Reference 49), for the generalized hypergeometric functions ${}_{3}F_{2}(a_{1}, a_{2}, a_{3}; b_{1}, b_{2}; 1)$ one might easily derive corresponding recurrence relations for the matrix elements presented in Eqs. (5.120)-(5.122), respectively (cf. Chapter 5.6).

In the following several elementary cases of the matrix $\mathbf{T}_{mn}^{(\ell)}$ are given, namely,

$$T_{mn}^{(2)} = \frac{1}{2} \int_{0}^{\infty} dt e^{-t} t^{3/2} L_{m}^{(3/2)}(t) L_{n}^{(5/2)}(t)$$

$$= \sum_{k=0}^{n} \frac{1}{2} \int_{0}^{\infty} dt e^{-t} t^{3/2} L_{m}^{(3/2)}(t) L_{k}^{(3/2)}(t)$$

$$= \sum_{k=0}^{n} \frac{\Gamma(m+5/2)}{2m!} \delta_{mk}, \qquad (5.123)$$

which yields

$$T_{mn}^{(2)} = \begin{cases} 0 & \text{for } m > n \\ \frac{\Gamma(m+5/2)}{2m!} & \text{for } m \le n \end{cases}$$
 (5.124)

as well as

$$T_{mn}^{(4)} = \frac{(-1)^m}{2m!} \sum_{k=0}^n (-1)^k \binom{n+9/2}{n-k} \frac{(k+1)\Gamma(k+7/2)}{\Gamma(k+2-m)},$$
 (5.125)

producing for $m \le n + 1$ the result [48]

$$T_{mn}^{(4)} = \frac{(-1)^m}{2m!} \sum_{k=m-1}^n (-1)^k \binom{n+9/2}{n-k} \frac{(k+1)\Gamma(k+7/2)}{\Gamma(k+2-m)}$$
$$= \frac{[5(n+1)-7m]\Gamma(m+5/2)}{4m!}, \tag{5.126}$$

whereas $T_{mn}^{(4)} = 0$ for m > n + 1. In deriving Eq. (5.125) the relation¹ $(-k)_n = (-1)^n k!/(k-n)!$, $k, n \in \mathbb{N}$ with $(z)_n$ being the Pochhammer symbol [47] has been used. It is worth noting that Eqs. (5.120) and (5.121) are especially simple if one of the parameters a_i in the generalized hypergeometric function ${}_3F_2$ is equal to zero since then, for example, ${}_3F_2(0, a_2, a_3; b_1, b_2; 1) = 1$.

5.5 Asymptotic expansions

The goal of this section is to study the asymptotic behavior of the matrix elements derived in the preceding sections for a small mass-ratio approximation. That is to say, the case when the mass ratio of test and field particles $m_a/m_b \ll 1$ will be considered which corresponds to electron-ion or ion-impurity collisions, respectively (the opposite limit, i.e. $m_a/m_b \gg 1$, is not examined but could be easily obtained by applying the same method to be described below).

The quantity $\gamma_{ab} = v_{ta}/v_{tb}$ representing the ratio of the thermal speeds reduces to $\gamma_{ab} = \sqrt{m_b/m_a}$ for equal species temperatures from which, in turn, it follows that γ_{ab} tends to infinity if $m_a/m_b \ll 1$.

All formulas listed below concerning the hypergeometric functions have been taken from Reference 47 where one can find further details and useful properties of these functions (see also Reference 49).

¹http://functions.wolfram.com/06.10.27.0004.01 [49]

The Gauss hypergeometric function is defined for |z| < 1 by the series

$$F(a,b;c;z) = F(b,a;c;z) = \sum_{n=0}^{\infty} \frac{(a)_n(b)_n}{(c)_n} \frac{z^n}{n!},$$
 (5.127)

where $(z)_n$ denotes Pochhammer's symbol,

$$(z)_0 = 1 (5.128)$$

$$(z)_n = z(z+1)(z+2)\cdots(z+n-1) = \frac{\Gamma(z+n)}{\Gamma(z)}.$$
 (5.129)

For $z \to 0$ the hypergeometric function can be expressed as

$$F(a,b;c;z) = 1 + \frac{ab}{c}z + \frac{a(a+1)b(b+1)}{2c(c+1)}z^2 + \mathcal{O}(z^3).$$
 (5.130)

In Sections 5.2.1, 5.2.2 and 5.3.2 it has been shown that the matrix elements are proportional to hypergeometric functions of the form $F(a,b;c;\frac{\gamma^2}{1+\gamma^2})$. Since $\gamma^2/(1+\gamma^2) \to 1$ for $\gamma \to \infty$ such functions are not appropriate to analyze the asymptotic behavior of the matrix elements [cf. Eq. (5.130)]. First of all, one has to apply the following linear transformation formula relating the hypergeometric functions F(a,b;c;z) and F(a,b;c;1-z), respectively.

$$F(a,b;c;z) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}F(a,b;a+b-c+1;1-z) + (1-z)^{c-a-b}\frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)} \times F(c-a,c-b;c-a-b+1;1-z),$$
(5.131)

for $|\arg(1-z)| < \pi$. Each term of Eq. (5.131) has a pole when $c = a + b \pm m$, with $m = 0, 1, 2, \dots$ For m = 0 this case is covered by the relation

$$F(a,b;a+b;z) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^{\infty} \frac{(a)_n(b)_n}{(n!)^2} \Big[2\psi(n+1) - \psi(a+n) - \psi(b+n) - \ln(1-z) \Big] (1-z)^n,$$
 (5.132)

provided that $|\arg(1-z)| < \pi$ and |1-z| < 1, whereas for m = 1, 2, 3, ... one has

$$F(a,b;a+b+m;z) = \frac{\Gamma(m)\Gamma(a+b+m)}{\Gamma(a+m)\Gamma(b+m)} \sum_{n=0}^{m-1} \frac{(a)_n(b)_n}{n!(1-m)_n} (1-z)^n$$

$$-\frac{\Gamma(a+b+m)}{\Gamma(a)\Gamma(b)} (z-1)^m \sum_{n=0}^{\infty} \frac{(a+m)_n(b+m)_n}{n!(n+m)!} (1-z)^n \Big[\ln(1-z)$$

$$-\psi(n+1) - \psi(n+m+1) + \psi(a+n+m) + \psi(b+n+m) \Big], \quad (5.133)$$

as well as

$$F(a,b;a+b-m;z) = \frac{\Gamma(m)\Gamma(a+b-m)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^{m-1} \frac{(a-m)_n(b-m)_n}{n!(1-m)_n} (1-z)^{n-m} - \frac{(-1)^m\Gamma(a+b-m)}{\Gamma(a-m)\Gamma(b-m)} \sum_{n=0}^{\infty} \frac{(a)_n(b)_n}{n!(n+m)!} (1-z)^n \Big[\ln(1-z) - \psi(n+1) - \psi(n+m+1) + \psi(a+n) + \psi(b+n) \Big],$$
 (5.134)

if $|\arg (1-z)| < \pi$ and |1-z| < 1. Here, $\psi(z)$ is the psi (or digamma) function [47] defined as

$$\psi(z) = \frac{\mathrm{d}}{\mathrm{d}z} \ln \Gamma(z), \tag{5.135}$$

with

$$\psi(1) = -\gamma \tag{5.136}$$

$$\psi(1/2) = -\gamma - 2\ln 2, \tag{5.137}$$

where γ designates Euler's constant, and which obeys the recurrence formula

$$\psi(z+1) = \psi(z) + \frac{1}{z}.$$
 (5.138)

5.5.1 Differential part

In Sections (5.2.1) and (5.2.2) the matrix elements with respect to the test particle operator have been derived in the form

$$\hat{\nu}_{mm'}^{ab}(\gamma_{ab}) = \sum_{j=0}^{m+m'} X_{mm'}^{(j)} p_{\nu}^{(j)}(\gamma_{ab})$$
 (5.139)

$$\hat{D}_{mm'}^{ab}(\gamma_{ab}) = \sum_{j=0}^{m+m'} Y_{mm'}^{(j)} p_D^{(j)}(\gamma_{ab}), \qquad (5.140)$$

where

$$p_{\nu}^{(j)}(\gamma) = \frac{j!}{\gamma(1+\gamma^2)^j} \left[F(1,j+1;\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) - F(1,j;\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) \right]$$
 (5.141)

$$p_D^{(j)}(\gamma) = \frac{j!}{\gamma(1+\gamma^2)^j} \left[\frac{F(1,j+1;\frac{3}{2};\frac{\gamma^2}{1+\gamma^2})}{(1+\gamma^2)} - F(1,j;\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) \right]. \quad (5.142)$$

Upon introducing the expansion parameter z

$$z \equiv \frac{1}{1 + \gamma_{ab}^2}, \qquad \gamma_{ab} = \frac{(1 - z)^{1/2}}{z^{1/2}}$$
 (5.143)

and in accordance with Eq. (5.131) the hypergeometric functions appearing in Eqs. (5.141) and (5.142) can be transformed to

$$F(1,b;\frac{3}{2};1-z) = \frac{F(1,b;b+\frac{1}{2};z)}{(1-2b)} + \frac{\Gamma(3/2)\Gamma(b-1/2)}{\Gamma(b)} \frac{z^{1/2-b}}{(1-z)^{1/2}}, \quad (5.144)$$

where the elementary case

$$F(a,b;b;z) = (1-z)^{-a}$$
(5.145)

has been utilized [47].

By means of

$$F(1,j;j+\frac{1}{2};z) = 1 + \frac{j}{(j+1/2)}z + \mathcal{O}(z^2), \tag{5.146}$$

which has been obtained from Eq. (5.130), and after using

$$\frac{1}{\gamma(1+\gamma^2)^j} = \frac{z^{j+1/2}}{(1-z)^{1/2}} \tag{5.147}$$

$$= z^{j+1/2} + \frac{1}{2}z^{j+3/2} + \mathcal{O}(z^{j+5/2}), \qquad (5.148)$$

as well as Eq. (5.144) it follows that the function $p_{\nu}^{(j)}$ may be rewritten in terms of expansion parameter z as

$$p_{\nu}^{(j)}(z) = j! z^{j} \left\{ \frac{z^{1/2}}{(1-z)^{1/2}} \left[\frac{F(1,j+1;j+\frac{3}{2};z)}{1-2(j+1)} - \frac{F(1,j;j+\frac{1}{2};z)}{1-2j} \right] \right\} + \frac{\sqrt{\pi}}{2} \Gamma(j-1/2) \frac{(j-1/2-jz)}{(1-z)}.$$
(5.149)

Here, Eq. (5.149) may be expanded with the help of MAPLE yielding the result

$$p_{\nu}^{(j)}(z) = \frac{\sqrt{\pi}}{2} \Gamma(j+1/2) - \frac{2\Gamma(j+1)}{(1+2j)(1-2j)} z^{j+1/2} - \frac{\sqrt{\pi}}{4} \Gamma(j-1/2) z - \mathcal{O}(z^{j+3/2}),$$
 (5.150)

from which one obtains the pitch-angle scattering matrix elements as

$$\hat{\nu}_{mm'}^{ab} = \hat{\nu}_{mm'}^{a\infty} - \frac{16}{3\pi} \left[\frac{\Gamma(m+5/2)\Gamma(m'+5/2)}{m!m'!} \right]^{1/2} z^{1/2} + \mathcal{O}(z), \tag{5.151}$$

keeping only the first two expansion terms. The leading order term, $\hat{\nu}_{mm'}^{a\infty}$, is related to the case when infinitely heavy background ions are assumed and can be expressed as

$$\hat{\nu}_{mm'}^{a\infty} = \frac{\sqrt{\pi}}{5} \left[\frac{m!\Gamma(m'+5/2)}{m'!\Gamma(m+5/2)} \right]^{1/2} \left[5(m+1) - m' \right], \tag{5.152}$$

valid for $m \ge m' - 1$ (note that $\hat{\nu}_{mm'}^{a\infty} = \hat{\nu}_{m'm}^{a\infty}$).

For the energy scattering part one arrives at the expression

$$p_D^{(j)}(z) = j! z^j \left\{ \frac{z^{1/2}}{(1-z)^{1/2}} \left[z \frac{F(1,j+1;j+\frac{3}{2};z)}{1-2(j+1)} - \frac{F(1,j;j+\frac{1}{2};z)}{1-2j} \right] \right\} - \frac{\sqrt{\pi}}{4} \Gamma(j-1/2) \frac{z}{(1-z)}, \quad (5.153)$$

resulting, again by using MAPLE, in the expansion formula

$$p_D^{(j)}(z) \approx -\frac{\sqrt{\pi}}{4}\Gamma(j-1/2)z + \mathcal{O}(z^{j+1/2}).$$
 (5.154)

The corresponding matrix elements become

$$\hat{D}_{mm'}^{ab} = \frac{3\sqrt{\pi}}{2} \left[\frac{m!m'!}{\Gamma(m+5/2)\Gamma(m'+5/2)} \right]^{1/2} c_{mm'} z + \mathcal{O}(z^{3/2}), \tag{5.155}$$

provided that m' > 0 (recalling that \hat{D}_{m0}^{ab} is identically zero), with the coefficients

$$c_{mm'} = \begin{cases} \frac{8}{105} \frac{m'\Gamma(m'+7/2)}{m'!} & \text{for } m' \le m+1\\ \frac{\Gamma(m+5/2)}{m!} \left[\frac{m'(m'+1)}{3} - \frac{2mm'}{5} + \frac{m(m-1)}{7} \right] & \text{for } m \le m'+1 \end{cases}$$
(5.156)

Therefore, it will be justified neglecting the contributions from background particles to $\hat{D}_{mm'}^{ab}$ assuming $m_a/m_b \ll 1$ (for example, the electron-proton mass ratio is approximately 1/1836).

5.5.2 Integral part

According to Eq. (5.101) the matrix elements of the field particle operator in the Burnett function basis are given as

$$\hat{I}_{nn'}^{(\ell)}(\gamma_{ab}) = \frac{3}{4\pi^{3/2}} \frac{(2n'+\ell)\Gamma(n'+\ell+1/2)}{\Gamma(n'+1)\Gamma(\ell+3/2)} \frac{\gamma_{ab}^{\ell-1}}{(1+\gamma_{ab}^2)^{\ell/2+1}} \times \sum_{k=0}^{n} \frac{(-1)^k}{k!} \binom{n+1/2}{n-k} \frac{\Gamma(\ell/2+k+2)}{(1+\gamma_{ab}^2)^k} P_{n'}^{(\ell)}(k,\gamma_{ab}), (5.157)$$

valid for n' > 0, and where

$$P_{n'}^{(\ell)}(k,\gamma) = F(1-n',\frac{\ell}{2}+k+2;\ell+\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) \\
-\frac{(2n'+\ell-1)}{(2n'+2\ell-1)(1+\gamma^2)}F(2-n',\frac{\ell}{2}+k+2;\ell+\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}). (5.158)$$

The quantity to be expanded in z is

$$\frac{\gamma_{ab}^{\ell-1}}{(1+\gamma_{ab}^2)^{\ell/2+1+k}} \mathcal{P}_{n'}^{(\ell)}(k,\gamma_{ab}) = z^{k+3/2} (1-z)^{\ell/2-1/2} \mathcal{P}_{n'}^{(\ell)}(k,z), \tag{5.159}$$

where the function $P_{n'}^{(\ell)}(k,z)$ implies the transformed hypergeometric series [cf. Eq. (5.131)]

$$F(a, \frac{\ell}{2} + k + 2; \ell + \frac{3}{2}; 1 - z) = \frac{\Gamma(\ell + 3/2)\Gamma(\ell/2 - 1/2 - k - a)}{\Gamma(\ell + 3/2 - a)\Gamma(\ell/2 - 1/2 - k)} \times F(a, \frac{\ell}{2} + k + 2; a + k - \frac{\ell - 3}{2}; z) + z^{\ell/2 - 1/2 - k - a} \frac{\Gamma(\ell + 3/2)\Gamma(a + k + 1/2 - \ell/2)}{\Gamma(a)\Gamma(\ell/2 + k + 2)} \times F(\ell + \frac{3}{2} - a, \frac{\ell - 1}{2} - k; \frac{\ell + 1}{2} - k - a; z),$$
 (5.160)

for a = 1 - n' and a = 2 - n', respectively.

The poles appearing in Eq. (5.160) for n' = 0 and n' = 1, assuming odd values for ℓ , are calculated from Eqs. (5.132)-(5.134). One arrives at the following logarithmic cases retaining only low order terms with regard to expansion parameter z.

$$F(1, b; b+1; 1-z) = b [\psi(1) - \psi(b) - \ln z] + b^2 [\psi(2) - \psi(b+1) - \ln z] z + \mathcal{O}(z^2), \quad (5.161)$$

$$F(2,b;b+2;1-z) = b(b+1) [\psi(1) - 1 - \psi(b) - \ln z] + b^{2}(b+1) [2\psi(2) - 1 - 2\psi(b+1) - 2\ln z] z + \mathcal{O}(z^{2}), \quad (5.162)$$

$$F(1,b;b+1+m;1-z) = \frac{(b+m)}{m} \sum_{n=0}^{m-1} \frac{(b)_n}{(1-m)_n} z^n$$

$$-\frac{(-1)^m \Gamma(b+1+m)}{\Gamma(b)m!} z^m \Big\{ \ln z - \psi(1) + \psi(b+m)$$

$$+ (b+m) \left[\ln z - \psi(2) + \psi(b+m+1) \right] z + \mathcal{O}(z^2) \Big\}, \quad (5.163)$$

$$F(2,b;b+2+m;1-z) = \frac{(b+m)(b+m+1)}{m(m+1)} \sum_{n=0}^{m-1} \frac{(n+1)(b)_n}{(1-m)_n} z^n$$

$$-\frac{(-1)^m \Gamma(b+2+m)}{\Gamma(b)m!} z^m \left\{ \ln z - \psi(1) + \psi(b+m) + \frac{1}{(m+1)} + \frac{(m+2)(b+m)}{(m+1)} \left[\ln z - \psi(2) + \psi(b+m+1) + \frac{1}{(m+2)} \right] z + \mathcal{O}(z^2) \right\},$$

$$(5.164)$$

$$F(1,b;b+1-m;1-z) = \frac{\Gamma(m)\Gamma(b+1-m)}{\Gamma(b)} \sum_{n=0}^{m-1} \frac{(b-m)_n}{n!} z^{n-m}$$
$$-\frac{(-1)^m(b-m)}{\Gamma(1-m)m!} \left\{ \ln z - \psi(m+1) + \psi(b) + \frac{b}{(m+1)} \left[\ln z - \psi(m+2) + \psi(b+1) \right] z + \mathcal{O}(z^2) \right\}, \quad (5.165)$$

and

$$F(2,b;b+2-m;1-z) = \frac{\Gamma(m)\Gamma(b+2-m)}{\Gamma(b)} \sum_{n=0}^{m-1} \frac{(2-m)_n(b-m)_n}{(1-m)_n n!} z^{n-m}$$

$$-\frac{(-1)^m(b-m)(b-m+1)}{\Gamma(2-m)m!} \left\{ \ln z - \psi(m+1) + \psi(b) + 1 + \frac{b}{(m+1)} \left[2\ln z - 2\psi(m+2) + 2\psi(b+1) + 1 \right] z + \mathcal{O}(z^2) \right\}. (5.166)$$

Keeping only leading order terms, it follows from Eqs. (5.163)-(5.166) that,

$$zF(1,b;b+1+m;1-z) = \frac{(b+m)}{m}z + \begin{cases} \mathcal{O}(z^2 \ln z) & \text{for } m=1\\ \mathcal{O}(z^2) & \text{for } m \ge 2, \end{cases}$$
 (5.167)

$$zF(2,b;b+2+m;1-z) = \frac{(b+m)(b+m+1)}{m(m+1)}z + \begin{cases} \mathcal{O}(z^2 \ln z) & \text{for } m=1\\ \mathcal{O}(z^2) & \text{for } m \ge 2, \end{cases}$$
(5.168)

$$zF(1,b;b+1-m;1-z) = \frac{\Gamma(m)\Gamma(b+1-m)}{\Gamma(b)}z^{1-m} + \begin{cases} 0 & \text{for } m=1\\ \mathcal{O}(z^{2-m}) & \text{for } m \ge 2, \end{cases}$$
(5.169)

as well as

$$zF(2, b; b + 2 - m; 1 - z)$$

$$= \frac{\Gamma(m)\Gamma(b + 2 - m)}{\Gamma(b)} z^{1 - m} + \begin{cases} \mathcal{O}(z \ln z) & \text{for } m = 1\\ 0 & \text{for } m = 2 \end{cases} (5.170)$$

$$\mathcal{O}(z^{2 - m}) & \text{for } m \ge 3.$$

An elaborated derivation of the expansion of the matrix elements is not given here as it is straightforward though rather tedious. Hence, simply the results are listed below which have essentially been obtained by means of MAPLE [48].

$n' \le 1$, even ℓ

Recalling Eq. (5.157) one immediately obtains for n'=0 and $\ell=0$ the result

$$\hat{I}_{n0}^{(0)}(z) \equiv 0. \tag{5.171}$$

 $n' = 0, \ \ell = 2$:

$$\hat{I}_{n0}^{(2)}(z) = \begin{cases} \frac{15}{16\pi^{1/2}} z + \mathcal{O}(z^{3/2}) & \text{for } n = 0\\ \frac{9}{8\pi^{1/2}} z + \mathcal{O}(z^{3/2}) & \text{for } n \ge 1 \end{cases}$$
 (5.172)

 $n' = 0, \ \ell > 4$:

$$\hat{I}_{n0}^{(\ell)}(z) = \frac{3}{2\pi^{3/2}} \frac{\ell\Gamma(\ell/2+2)}{(\ell-3)} {n+1/2 \choose n} z^{3/2} + \begin{cases} \mathcal{O}(z^2) & \text{for } \ell = 4\\ \mathcal{O}(z^{5/2}) & \text{for } \ell > 6 \end{cases}$$
(5.173)

 $n' = 1, \ \ell = 0$:

$$\hat{I}_{n1}^{(0)}(z) = \begin{cases} -\frac{3}{8\pi^{1/2}}z + \mathcal{O}(z^{3/2}) & \text{for } n = 0\\ \frac{3}{2\pi^{3/2}} {n+1/2 \choose n} z^{3/2} + \mathcal{O}(z^{5/2}) & \text{for } n \ge 1 \end{cases}$$
 (5.174)

 $n' = 1, \ \ell > 2$:

$$\hat{I}_{n1}^{(\ell)}(z) = \frac{3(\ell+2)}{4\pi^{3/2}} \Gamma(\ell/2+2) \binom{n+1/2}{n} z^{3/2} + \begin{cases} \mathcal{O}(z^2) & \text{for } \ell=2\\ \mathcal{O}(z^{5/2}) & \text{for } \ell \ge 4 \end{cases}$$
(5.175)

 $n' \leq 1$, odd ℓ

 $n' = 0, \ \ell = 3$:

$$\hat{I}_{n0}^{(3)}(z) = \frac{135}{32\pi} {n+1/2 \choose n} \left[\frac{24n}{5(2n+1)} - \frac{52}{15} - \psi(n+1/2) - \gamma - \ln z \right] z^{3/2} + \mathcal{O}(z^{5/2} \ln z)$$
 (5.176)

 $n' = 0, \ \ell \ge 5$:

$$\hat{I}_{n0}^{(\ell)}(z) = \frac{3}{2\pi^{3/2}} \binom{n+1/2}{n} \frac{\ell\Gamma(\ell/2+2)}{(\ell-3)} z^{3/2} + \begin{cases} \mathcal{O}(z^{5/2} \ln z) & \text{for } \ell = 5\\ \mathcal{O}(z^{5/2}) & \text{for } \ell \geq 7 \end{cases}$$
(5.177)

 $n' = 1, \ \ell > 3$:

$$\hat{I}_{n1}^{(\ell)}(z) = \frac{3}{4\pi^{3/2}} (\ell+2) \Gamma(\ell/2+2) \binom{n+1/2}{n} z^{3/2} + \begin{cases} \mathcal{O}(z^{5/2} \ln z) & \text{for } \ell = 3\\ \mathcal{O}(z^{5/2}) & \text{for } \ell \ge 5. \end{cases}$$
(5.178)

$$n' > 2$$
, $\ell > 0$

For the case when the parameter $n' \geq 2$ the hypergeometric functions reduce to a polynomial of degree n' in the argument z. Thus, by using Eqs. (5.157), (5.160) and (5.130) the behavior of the matrix elements for small values of z is characterized by the expression

$$\hat{I}_{nn'}^{(\ell)}(z) = \frac{3}{4\pi^{3/2}} {n+1/2 \choose n} \frac{\Gamma(\ell/2+2)}{\Gamma(\ell/2-1/2)} \times \frac{(2n'+\ell)\Gamma(\ell/2+n'-3/2)}{n'!} z^{3/2} + \mathcal{O}(z^{5/2}).$$
 (5.179)

$$n' \geq 0$$
, $\ell = 1$

If the parameter ℓ is equal to one the expansion of the corresponding matrix elements may be obtained by means of Eq. (5.109). It follows that

$$\hat{I}_{nn'}^{(1)}(z) = \frac{3}{16\pi^{3/2}} (2n'+1)(4nn'+2n+2n'-1) \times \frac{\Gamma(n+n'-1/2)}{n!n'!} z^{n'+1/2} + \mathcal{O}(z^{n'+3/2}).$$
 (5.180)

Consequently, from the above analysis of asymptotic behavior of the field particle collision matrix elements, it is justified neglecting the contributions from background ions to $\hat{I}_{nn'}^{(\ell)}$, and $\hat{I}_{mm'}^{(\ell)}$, respectively, as well provided that $m_a/m_b \ll 1$ is assumed.

5.6 Recurrence relations

The matrix elements derived in preceding sections have been mainly presented as sum of functions involving Gauss' hypergeometric series [see, e.g., Eqs. (5.38), (5.56), (5.71), and (5.101)]. These relations are not in a form well suitable for numerical evaluation. Thus, it would be highly desirable to have recurrence relations which makes them easy to calculate and, first of all, allow for much faster numerical evaluation of the matrix elements than a direct computation of the analytical equations. In the following sections corresponding recurrence relations for the collision matrix elements as well as the transformation matrix are derived based on standard properties of associated Laguerre polynomials and recurrence identities of hypergeometric functions, respectively, which can be found in References 29, 47, and 49.

5.6.1 Source term elements $a_m^{(i)}$

The source term matrix elements (see Chapter 5.1)

$$a_m^{(i)} \equiv (\varphi_m, x^{2i-1-5\delta_{3i}}), \qquad i = 1, 2, 3$$
 (5.181)

are defined recursively by the recurrence relation

$$a_{m+1}^{(i)} = \frac{[m-i+(1+5\delta_{3i})/2]}{\sqrt{(m+1)(m+5/2)}} a_m^{(i)},$$
 (5.182)

and the initial values

$$a_0^{(1)} = \frac{2}{\pi} \sqrt{\frac{2}{3}}, \qquad a_0^{(2)} = \frac{2}{\pi} \sqrt{6}, \qquad a_0^{(3)} = \frac{1}{2} \sqrt{\frac{3}{2\pi}}.$$
 (5.183)

5.6.2 Pitch-angel scattering part

Recalling Eq. (5.24), where the matrix elements $\hat{\nu}_{mm'}^{ab}$ have been defined by the integral

$$\hat{\nu}_{mm'}^{ab} = \frac{3\sqrt{\pi}}{4\sqrt{h_m h_{m'}} \gamma} \int_{0}^{\infty} dy e^{-(y^2/\gamma^2)} L_m^{(3/2)}(y^2/\gamma^2) \times L_{m'}^{(3/2)}(y^2/\gamma^2) [\phi(y) - G(y)], \quad (5.184)$$

it immediately follows that

$$\hat{\nu}_{mm'}^{ab} = \hat{\nu}_{m'm}^{ab}. \tag{5.185}$$

Multiplying Eq. (5.184) (for $m \to m+1$) by m+1 and with the help of various properties of associated Laguerre polynomials [29],

$$(m+1)L_{m+1}^{(3/2)}(x) = (2m+5/2-x)L_m^{(3/2)}(x) - (m+3/2)L_{m-1}^{(3/2)}(x)$$
(5.186)

$$xL_{m'}^{(3/2)}(x) = (2m' + 5/2)L_{m'}^{(3/2)}(x) - (m' + 1)L_{m'+1}^{(3/2)}(x) - (m' + 3/2)L_{m'-1}^{(3/2)}(x),$$

$$(5.187)$$

one arrives at the recurrence relation

$$\sqrt{(m+1)(m+5/2)}\hat{\nu}_{m+1m'} =$$

$$-\sqrt{m(m+3/2)}\hat{\nu}_{m-1m'} + 2(m-m')\hat{\nu}_{mm'} + \sqrt{m'(m'+3/2)}\hat{\nu}_{mm'-1} + \sqrt{(m'+1)(m'+5/2)}\hat{\nu}_{mm'+1}, \qquad (5.188)$$

where

$$h_m = \frac{\Gamma(m+5/2)}{2m!} {(5.189)}$$

$$h_{m+1} = \frac{(m+5/2)}{(m+1)}h_m, (5.190)$$

with the initial value $h_0 = 3\sqrt{\pi}/8$, has been used. Here, Eq. (5.188) yields, with m = 0,

$$\sqrt{5}\hat{\nu}_{1m'} = \sqrt{m'(2m'+3)}\hat{\nu}_{0m'-1} - 2\sqrt{2}m'\hat{\nu}_{0m'} + \sqrt{(m'+1)(2m'+5)}\hat{\nu}_{0m'+1},$$
(5.191)

valid for $m' \geq 1$, whereas the recurrence relation for $\hat{\nu}_{0m'}$ remains to be calculated. Having started from Eq. (5.184) with m = 0, that is,

$$\hat{\nu}_{0m'} = \frac{3\sqrt{\pi}}{4\sqrt{h_0 h_{m'} \gamma}} \int_0^\infty \mathrm{d}y e^{-(y^2/\gamma^2)} L_{m'}^{(3/2)}(y^2/\gamma^2) [\phi(y) - G(y)], \qquad (5.192)$$

one may define the auxiliary quantities

$$p_{m'} \equiv \int_{0}^{\infty} dy e^{-(y^2/\gamma^2)} L_{m'}^{(3/2)}(y^2/\gamma^2) \phi(y)$$
 (5.193)

$$g_{m'} \equiv \int_{0}^{\infty} dy e^{-(y^2/\gamma^2)} L_{m'}^{(3/2)}(y^2/\gamma^2) G(y),$$
 (5.194)

in which the error and the Chandrasekhar function, respectively, satisfy the following equations,

$$\int dy \phi(y) = y\phi(y) + \frac{e^{-y^2}}{\sqrt{\pi}}$$
(5.195)

$$\int \mathrm{d}y G(y) = -\frac{\phi(y)}{2y}.$$
(5.196)

Integrating Eq. (5.193) by parts, remembering Eq. (5.195), gives

$$p_{m'} = \left[e^{-(y^2/\gamma^2)} L_{m'}^{(3/2)}(y^2/\gamma^2) \left(y\phi(y) + \frac{e^{-y^2}}{\sqrt{\pi}} \right) \right] \Big|_0^{\infty}$$

$$+ \int_0^{\infty} dy \left[y\phi(y) + \frac{e^{-y^2}}{\sqrt{\pi}} \right] e^{-(y^2/\gamma^2)} \frac{2y}{\gamma^2} L_{m'}^{(5/2)}(y^2/\gamma^2), \quad (5.197)$$

where in the second term on the RHS of last equation the following identities [29] of associated Laguerre polynomials have been utilized,

$$\left[L_{m'}^{(\alpha)}(x)\right]' \equiv \frac{\mathrm{d}}{\mathrm{d}x} L_{m'}^{(\alpha)}(x) = -L_{m'-1}^{(\alpha+1)}(x) \tag{5.198}$$

$$L_{m'}^{(\alpha-1)}(x) = L_{m'}^{(\alpha)}(x) - L_{m'-1}^{(\alpha)}(x)$$
 (5.199)

$$xL_{m'}^{(\alpha+1)}(x) = (m' + \alpha + 1)L_{m'}^{(\alpha)}(x) - (m' + 1)L_{m'+1}^{(\alpha)}(x), \quad (5.200)$$

and the first term on the RHS of Eq. (5.197), using

$$L_{m'}^{(\alpha)}(0) = \binom{m' + \alpha}{m'},\tag{5.201}$$

adds up to

$$\left[e^{-(y^2/\gamma^2)} L_{m'}^{(3/2)}(y^2/\gamma^2) \left(y\phi(y) + \frac{e^{-y^2}}{\sqrt{\pi}} \right) \right] \Big|_0^{\infty} = -\frac{1}{\sqrt{\pi}} {m' + 3/2 \choose m'}. \quad (5.202)$$

Thus, Eq.(5.193) can be recast to the relation

$$2(m'+1)p_{m'+1} = -\frac{1}{\sqrt{\pi}} {m'+3/2 \choose m'} + 2(m'+2)p_{m'} + \frac{1}{\sqrt{\pi}} \int_{0}^{\infty} dz e^{-z(1+\gamma^2)} L_{m'}^{(5/2)}(z), \qquad (5.203)$$

with $z = y^2/\gamma^2$ and where again Eq. (5.200) has been used. Similarly, one obtains for the function $g_{m'}$,

$$g_{m'} = \left[-e^{-(y^2/\gamma^2)} L_{m'}^{(3/2)}(y^2/\gamma^2) \frac{\phi(y)}{2y} \right]_0^{\infty}$$

$$- \frac{1}{\gamma^2} \int_0^{\infty} dy e^{-(y^2/\gamma^2)} \phi(y) L_{m'}^{(5/2)}(y^2/\gamma^2), \qquad (5.204)$$

with

$$\left[-e^{-(y^2/\gamma^2)} L_{m'}^{(3/2)}(y^2/\gamma^2) \frac{\phi(y)}{2y} \right] \Big|_0^\infty = \frac{1}{\sqrt{\pi}} \binom{m' + 3/2}{m'}. \tag{5.205}$$

From the definition of the Chandrasekhar function G [see Eq. 5.21] the error function can be expressed by

$$\phi(y) = 2y^2 G(y) + \frac{2y}{\sqrt{\pi}} e^{-y^2}, \qquad (5.206)$$

which in turn may be substituted in Eq. (5.204) yielding, together with Eq. (5.200), the result

$$2(m'+1)g_{m'+1} = -\frac{1}{\sqrt{\pi}} {m'+3/2 \choose m'} + 2(m'+3)g_{m'} + \frac{1}{\sqrt{\pi}} \int_{0}^{\infty} dz e^{-z(1+\gamma^2)} L_{m'}^{(5/2)}(z).$$
 (5.207)

Next, subtracting Eqs. (5.203) and (5.207), one easily sees that the terms involving the binomial coefficients as well as the integrals with respect to z cancel out yielding

$$(m'+1)(p_{m'+1}-g_{m'+1}) = (m'+2)(p_{m'}-g_{m'}) - g_{m'}, (5.208)$$

from which, by means of Eqs. (5.192)-(5.194), one can infer that

$$\frac{4\gamma}{3\sqrt{\pi}}\sqrt{h_0h_{m'+1}}(m'+1)\hat{\nu}_{0m'+1} = \frac{4\gamma}{3\sqrt{\pi}}\sqrt{h_0h_{m'}}(m'+2)\hat{\nu}_{0m'} - g_{m'}. \quad (5.209)$$

This means that having found a recurrence relation for $g_{m'}$ results in a corresponding recurrence relation for $\hat{\nu}_{0m'}$.

The integral appearing in Eq. (5.207) may be evaluated applying [29]

$$\int_{0}^{\infty} dz e^{-sz} z^{\beta} L_n^{(\alpha)}(z) = \frac{\Gamma(\beta+1)\Gamma(n+\alpha+1)}{n!\Gamma(\alpha+1)s^{\beta+1}} F(-n,\beta+1;\alpha+1;\frac{1}{s}), \quad (5.210)$$

valid for Re $\beta > -1$ and Re s > 0, which leads to

$$\int_{0}^{\infty} dz e^{-z(1+\gamma^{2})} L_{m'}^{(5/2)}(z)$$

$$= \frac{1}{(1+\gamma^{2})} {m'+5/2 \choose m'} F(-m', 1; \frac{7}{2}; \frac{1}{1+\gamma^{2}})$$

$$= {m'+3/2 \choose m'} \left[1 - \frac{\gamma^{2}}{(1+\gamma^{2})} F(-m', 1; \frac{5}{2}; \frac{1}{1+\gamma^{2}})\right], (5.211)$$

where in the last equation a Gauss' relation for contiguous hypergeometric functions [47],

$$(c-a)zF(a,b;c+1;z) = cF(a,b-1;c;z) - c(1-z)F(a,b;c;z), \quad (5.212)$$

has been employed [noting that F(a, 0; c; z) = 1]. Substituting Eq. (5.211) into Eq. (5.207) gives rise to

$$2(m'+1)g_{m'+1} = 2(m'+3)g_{m'} - \frac{1}{\sqrt{\pi}} {m'+3/2 \choose m'} \frac{\gamma^2}{(1+\gamma^2)} F(-m', 1; \frac{5}{2}; \frac{1}{1+\gamma^2}). (5.213)$$

After using another Gauss' relation for F, namely

$$(c-a-b)F(a,b;c;z) = (c-a)F(a-1,b;c;z) - b(1-z)F(a,b+1;c;z), (5.214)$$

one obtains from Eq. (5.213) the desired recurrence relation for the quantity $g_{m'}$,

$$(m'+1)g_{m'+1} = \left[m'+3+\frac{m'\gamma^2}{(1+\gamma^2)}\right]g_{m'} - \frac{\gamma^2}{(1+\gamma^2)}\left[(m'+2)g_{m'-1}+\frac{1}{2\sqrt{\pi}}\binom{m'+1/2}{m'}\right]. (5.215)$$

Finally, by using Eqs. (5.209) and (5.215), one finds the following recurrence relation for the matrix elements $\hat{\nu}_{0m'}$ satisfying

$$\sqrt{(m'+1)(m'+2)(m'+5/2)(m'+7/2)}\hat{\nu}_{0m'+2} = \frac{\gamma^2}{(1+\gamma^2)} \left[\frac{3}{\sqrt{\pi}\gamma(2m'+3)} \sqrt{\frac{h_{m'}}{h_0}} + (m'+1)(m'+2) \sqrt{\frac{m'}{(m'+3/2)}} \hat{\nu}_{0m'-1} \right] - (m'+2) \left[m'+3 + \frac{2m'\gamma^2}{(1+\gamma^2)} \right] \hat{\nu}_{0m'} + \sqrt{(m'+1)(m'+5/2)} \times \left[2(m'+3) + \frac{m'\gamma^2}{(1+\gamma^2)} \right] \hat{\nu}_{0m'+1},$$
(5.216)

with the initial values

$$\hat{\nu}_{00}(\gamma) = \frac{2}{\sqrt{\pi}\gamma} \left[\frac{(1+\gamma^2)}{\gamma} \arctan \gamma - 1 \right]$$
 (5.217)

$$\hat{\nu}_{01}(\gamma) = \frac{2\sqrt{2}}{\sqrt{5\pi}\gamma} \left[\frac{(3+2\gamma^2)}{\gamma} \arctan \gamma - 3 \right]$$
 (5.218)

$$\hat{\nu}_{02}(\gamma) = \sqrt{\frac{2}{35}} \left[\frac{\gamma}{\sqrt{\pi}(1+\gamma^2)} - 6\hat{\nu}_{00}(\gamma) + 3\sqrt{10}\hat{\nu}_{01}(\gamma) \right], \quad (5.219)$$

where the last equation has been found from Eq. (5.216) with m'=0.

5.6.3 Matrix elements $\hat{\nu}_{mm'}^{a\infty}$

In Section 5.2.1 the matrix elements attached to pitch-angle scattering operator \mathcal{L} assuming infinitely heavy background ions have been found to be

$$\hat{\nu}_{mm'}^{a\infty} = \frac{\sqrt{\pi}}{5} \left[\frac{m!\Gamma(m'+5/2)}{m'!\Gamma(m+5/2)} \right]^{1/2} \left[5(m+1) - m' \right], \quad m \ge m' - 1, \quad (5.220)$$

remembering that $\hat{\nu}_{mm'}^{a\infty} = \hat{\nu}_{m'm}^{a\infty}$. Here, Eq. (5.220) gives

$$\hat{\nu}_{mm}^{a\infty} = \frac{\sqrt{\pi}}{5} (4m+5), \tag{5.221}$$

as well as the recurrence relation

$$\hat{\nu}_{m+1m'}^{a\infty} = \left(\frac{m+1}{m+5/2}\right)^{1/2} \frac{\left[5(m+2) - m'\right]}{\left[5(m+1) - m'\right]} \hat{\nu}_{mm'}^{a\infty},\tag{5.222}$$

with

$$\hat{\nu}_{m+1\,0}^{a\infty} = \frac{(m+2)}{\sqrt{(m+1)(m+5/2)}} \hat{\nu}_{m0}^{a\infty},\tag{5.223}$$

and initial value $\hat{\nu}_{00}^{a\infty} = \sqrt{\pi}$.

5.6.4 Energy scattering part

In accordance with Eq. (5.51) the matrix elements with respect to the energy scattering part of the test particle operator $C_{ab}^{D,v}$ are evaluated by

$$\hat{D}_{mm'} = \frac{3\sqrt{\pi}}{4\sqrt{h_m h_{m'}} \gamma} \int_0^\infty dy y L_m^{(3/2)}(y^2/\gamma^2) \times \frac{\partial}{\partial y} \left\{ G(y) e^{-y^2/\gamma^2} 2 \frac{y^2}{\gamma^2} \left[L_{m'}^{(3/2)}(y^2/\gamma^2) \right]' \right\}, \qquad (5.224)$$

from which one can directly see [since $L_0^{(3/2)}(y^2/\gamma^2)=1$] that

$$\hat{D}_{m0} \equiv 0. \tag{5.225}$$

A recurrence relation for the matrix elements $\hat{D}_{mm'}$ may be derived with the help of the quantity $d_{mm'}$ defined as

$$d_{mm'} = \int_{0}^{\infty} dy e^{-y^2/\gamma^2} L_m^{(3/2)}(y^2/\gamma^2) G(y) 2 \frac{y^2}{\gamma^2} \left[L_{m'}^{(3/2)}(y^2/\gamma^2) \right]', \qquad (5.226)$$

which obeys the recurrence relation

$$(m+1)d_{m+1m'} = (m'+3/2)d_{mm'-1} - (2m'-2m-1)d_{mm'} + m'd_{mm'+1} - (m+3/2)d_{m-1m'},$$
 (5.227)

where Eqs. (5.198)-(5.200) have been used. By means of MAPLE [48] one can show that $d_{mm'}$ can be expressed as a sum of matrix elements presented in Eq. (5.224) as follows

$$\frac{3\sqrt{\pi}}{4\gamma} d_{mm'} = -(2m+3) \sum_{k=0}^{m} \frac{\sqrt{h_k h_{m'}}}{(2k+1)(2k+3)} \hat{D}_{km'}.$$
 (5.228)

Substituting this relationship into Eq. (5.227) yields, together with Eqs. (5.189) and (5.190),

$$\frac{\sqrt{(m+1)(m+5/2)}}{(2m+3)}\hat{D}_{m+1m'} = \frac{1}{2}\hat{D}_{mm'} + (2m+3)\left\{\sum_{k=0}^{m} \sqrt{\frac{h_k}{h_m}} \frac{1}{(2k+1)(2k+3)} \times \left[m'\sqrt{\frac{(m'+5/2)}{(m'+1)}}\hat{D}_{km'+1} + \sqrt{m'(m'+3/2)}\hat{D}_{km'-1} - \left(2m' + \frac{6m+7}{2(2m+3)}\right)\hat{D}_{km'}\right]\right\},$$
(5.229)

from which one obtains, after some tedious but straightforward algebraic manipulation (by carrying out $\hat{D}_{m+1m'} - \hat{D}_{mm'}$ and rearranging terms), a recurrence relation for $\hat{D}_{mm'}$ in the form

$$\sqrt{(m+1)(m+5/2)} \frac{(2m+1)}{(2m+3)} \hat{D}_{m+1m'} = \sqrt{m'(m'+3/2)} \hat{D}_{mm'-1}
+ m' \sqrt{\frac{(m'+5/2)}{(m'+1)}} \hat{D}_{mm'+1} - \sqrt{m(m+3/2)} \hat{D}_{m-1m'}
+ \left[\frac{2(m+1)(4m^2+4m-1)}{(2m+1)(2m+3)} - 2m' \right] \hat{D}_{mm'}
- 2 \sum_{k=0}^{m-1} \sqrt{\frac{h_k}{h_m}} \frac{\hat{D}_{km'}}{(2k+1)(2k+3)},$$
(5.230)

if $m \ge 1$ and $m' \ge 1$, respectively. Here, Eq. (5.229) gives

$$\frac{\sqrt{5}}{3\sqrt{2}}\hat{D}_{1m'} = \sqrt{m'(m'+3/2)}\hat{D}_{0m'-1} - \left(2m' + \frac{2}{3}\right)\hat{D}_{0m'}$$

$$+ m' \sqrt{\frac{(m'+5/2)}{(m'+1)}} \hat{D}_{0m'+1}. \tag{5.231}$$

By virtue of Eq. (5.224) and after an integration by parts one gets for m' > 0, by using properties of the associated Laguerre polynomials [cf. Eqs. (5.198) and (5.200)],

$$\frac{4\gamma}{3\sqrt{\pi}}\sqrt{h_0h_{m'}}\hat{D}_{0m'} = (2m'+3)\int_0^\infty dy e^{(-y^2/\gamma^2)}G(y)L_{m'-1}^{(3/2)}(y^2/\gamma^2)
-2m'\int_0^\infty dy e^{(-y^2/\gamma^2)}G(y)L_{m'}^{(3/2)}(y^2/\gamma^2)
= (2m'+3)g_{m'-1} - 2m'g_{m'},$$
(5.232)

where Eq. (5.194) has been employed. This result may be expressed in terms of the matrix elements $\hat{\nu}_{0m'}$ [see Eq. (5.209) as well as Eqs. (5.189)-(5.190)] yielding for $m' \geq 1$,

$$\hat{D}_{0m'} = 2(m'+1)\sqrt{m'(m'+3/2)}\hat{\nu}_{0m'-1} - 2m'(2m'+7/2)\hat{\nu}_{0m'}
+2m'\sqrt{(m'+1)(m'+5/2)}\hat{\nu}_{0m'+1}.$$
(5.233)

5.6.5 Transformation matrix

In the following a recurrence relation for the quantity

$$T_{mn}^{(\ell)} \equiv \frac{1}{2} \int_{0}^{\infty} dt e^{-t} t^{(\ell+1)/2} L_m^{(3/2)}(t) L_n^{(\ell+1/2)}(t), \qquad (5.234)$$

as well as for the transformation matrix $\phi_{mn}^{(\ell)} \equiv T_{mn}^{(\ell)}/(\pi^{3/4}\sqrt{h_m})$ between the two sets of basis functions φ_m and $B_n^{(\ell)}$, respectively, will be derived. From Eq. (5.234), by replacing m with m+1 and upon multiplication with m+1, one gets the expression

$$(m+1)\mathbf{T}_{m+1n}^{(\ell)} = (2m-2n-\ell+1)\mathbf{T}_{mn}^{(\ell)} - (m+3/2)\mathbf{T}_{m-1n}^{(\ell)} + (n+1)\mathbf{T}_{mn+1}^{(\ell)} + (n+\ell+1/2)\mathbf{T}_{mn-1}^{(\ell)},$$
 (5.235)

if $m \ge 1$ and $n \ge 1$, where the following identities of associated Laguerre polynomials [29] have been used,

$$(m+1)L_{m+1}^{(3/2)} = (2m+5/2)L_m^{(3/2)} - (m+3/2)L_{m-1}^{(3/2)} - tL_m^{(3/2)} (5.236)$$

$$tL_n^{(\ell+1/2)} = (2n+\ell+3/2)L_n^{(\ell+1/2)} - (n+1)L_{n+1}^{(\ell+1/2)}$$

$$-(n+\ell+1/2)L_{n-1}^{(\ell+1/2)}. (5.237)$$

With the help of

$$tL_n^{(\ell+5/2)} = (n+\ell+5/2)L_n^{(\ell+3/2)} - (n+1)L_{n+1}^{(\ell+3/2)}$$
(5.238)

and

$$L_n^{(\alpha+1)} = \sum_{k=0}^n L_k^{(\alpha)},\tag{5.239}$$

it follows from Eq. (5.234), with $\ell \to \ell + 2$, that

$$T_{mn}^{(\ell+2)} = \frac{1}{2} \int_{0}^{\infty} dt e^{-t} t^{(\ell+3)/2} L_{m}^{(3/2)}(t) L_{n}^{(\ell+5/2)}(t)$$

$$= (n+\ell+5/2) \sum_{k=0}^{n} T_{mk}^{(\ell)} - (n+1) \sum_{k=0}^{n+1} T_{mk}^{(\ell)}$$

$$= (\ell+3/2) \sum_{k=0}^{n} T_{mk}^{(\ell)} - (n+1) T_{mn+1}^{(\ell)}, \qquad (5.240)$$

which, in turn, leads with $n \to n+1$ to

$$T_{mn+1}^{(\ell+2)} = (\ell+3/2) \sum_{k=0}^{n+1} T_{mk}^{(\ell)} - (n+2) T_{mn+2}^{(\ell)}$$
$$= T_{mn}^{(\ell+2)} + (n+\ell+5/2) T_{mn+1}^{(\ell)} - (n+2) T_{mn+2}^{(\ell)}. \quad (5.241)$$

By using Eq. (5.119) it immediately follows that

$$T_{0n}^{(\ell)} = \frac{\Gamma(\ell/2 + 3/2)}{2n!} (\ell/2)_n , \qquad (5.242)$$

with $(z)_n = \Gamma(z+n)/\Gamma(z)$ indicating the Pochhammer symbol [47] and, accordingly,

$$T_{0n+1}^{(\ell)} = \frac{(n+\ell/2)}{(n+1)} T_{0n}^{(\ell)}.$$
 (5.243)

Likewise, from Eq. (5.119) one obtains

$$T_{1n}^{(\ell)} = \left[5/2 - \frac{(\ell+3)(\ell-2)}{2(2n-2+\ell)} \right] T_{0n}^{(\ell)}, \tag{5.244}$$

leading to

$$T_{1n+1}^{(\ell)} = \frac{5(2n+\ell) - (\ell+3)(\ell-2)}{4(n+1)} T_{0n}^{(\ell)}, \tag{5.245}$$

where Eq. (5.243) has been utilized.

From similar considerations regarding the parameter m one obtains the formulas [see Eq. (5.118)]

$$T_{m0}^{(\ell)} = \frac{\Gamma(\ell/2 + 3/2)}{2m!} (1 - \ell/2)_m$$
 (5.246)

$$T_{m+10}^{(\ell)} = \frac{(m-\ell/2+1)}{(m+1)} T_{m0}^{(\ell)},$$
 (5.247)

as well as

$$T_{m1}^{(\ell)} = \left[\ell + 3/2 + \frac{\ell(\ell+3)}{2(2m-\ell)}\right] T_{m0}^{(\ell)}, \tag{5.248}$$

and, by using Eq. (5.247),

$$T_{m+11}^{(\ell)} = \frac{(2\ell+3)(2m+2-\ell) + \ell(\ell+3)}{4(m+1)} T_{m0}^{(\ell)}.$$
 (5.249)

The initial values follow directly from Eqs. (5.242) or (5.246), respectively,

$$T_{00}^{(\ell)} = \frac{1}{2}\Gamma(\ell/2 + 3/2) \tag{5.250}$$

$$T_{00}^{(0)} = \frac{\sqrt{\pi}}{4}, \qquad T_{00}^{(1)} = \frac{1}{2}.$$
 (5.251)

Upon using Eqs. (5.235) and (5.111) along with Eqs. (5.189) and (5.190) one gets

$$\sqrt{(m+1)(m+5/2)}\phi_{m+1n}^{(\ell)} = (2m-2n-\ell+1)\phi_{mn}^{(\ell)}
- \sqrt{m(m+3/2)}\phi_{m-1n}^{(\ell)} + (n+1)\phi_{mn+1}^{(\ell)}
+ (n+\ell+1/2)\phi_{mn-1}^{(\ell)},$$
(5.252)

for $m \ge 0$ and $n \ge 1$. A recursion formula with respect to parameter ℓ follows directly from Eqs. (5.240) and (5.241), that is

$$\phi_{mn}^{(\ell+2)} = (\ell+3/2) \sum_{k=0}^{n} \phi_{mk}^{(\ell)} - (n+1)\phi_{mn+1}^{(\ell)}, \qquad (5.253)$$

as well as

$$\phi_{mn+1}^{(\ell+2)} = \phi_{mn}^{(\ell+2)} + (n+\ell+5/2)\phi_{mn+1}^{(\ell)} - (n+2)\phi_{mn+2}^{(\ell)}.$$
 (5.254)

In order to be able to use Eq. (5.252) one must provide corresponding relations for the elements $\phi_{0n}^{(\ell)}$ and $\phi_{m0}^{(\ell)}$, as well as $\phi_{1n}^{(\ell)}$ and $\phi_{m1}^{(\ell)}$, respectively, which can be calculated from Eqs. (5.243) and (5.247),

$$\phi_{0n+1}^{(\ell)} = \frac{(n+\ell/2)}{(n+1)}\phi_{0n}^{(\ell)} \tag{5.255}$$

$$\phi_{m+10}^{(\ell)} = \frac{(m-\ell/2+1)}{\sqrt{(m+1)(m+5/2)}} \phi_{m0}^{(\ell)}, \tag{5.256}$$

and accordingly [see Eqs. (5.245) and (5.249)]

$$\phi_{1n+1}^{(\ell)} = \frac{\left[5(2n+\ell) - (\ell+3)(\ell-2)\right]\sqrt{2}}{4(n+1)\sqrt{5}}\phi_{0n}^{(\ell)}$$
 (5.257)

$$\phi_{m+11}^{(\ell)} = \frac{(2\ell+3)(2m+2-\ell) + \ell(\ell+3)}{4\sqrt{(m+1)(m+5/2)}}\phi_{m0}^{(\ell)}, \qquad (5.258)$$

with the initial values

$$\phi_{00}^{(0)} = \frac{1}{\sqrt{6\pi}}, \qquad \phi_{00}^{(1)} = \frac{\sqrt{2}}{\sqrt{3\pi}},$$
 (5.259)

obtained from

$$\phi_{00}^{(\ell)} = \sqrt{\frac{2}{3}} \, \frac{\Gamma(\ell/2 + 3/2)}{\pi}.\tag{5.260}$$

An additional recurrence relation for $T_{mn}^{(\ell)}$ may be derived starting from Eq. (5.120),

$$T_{mn}^{(\ell)} = \frac{\Gamma(\ell/2+3/2)\Gamma(m+1-\ell/2)}{2m!\Gamma(1-\ell/2)} \times {\binom{n+\ell+1/2}{n}}_{3}F_{2}(-n,\frac{\ell}{2},\frac{\ell+3}{2};\ell+\frac{3}{2},\frac{\ell}{2}-m;1), \quad (5.261)$$

and utilizing the following recurrence identity for consecutive neighbors,

$$_{3}F_{2}(a, a2, a3; b_{1}, b_{2}; z) = (B_{1} + C_{1}z) \,_{3}F_{2}(a + 1, a2, a3; b_{1}, b_{2}; z)$$

 $+ (B_{2} + C_{2}z) \,_{3}F_{2}(a + 2, a2, a3; b_{1}, b_{2}; z)$
 $+ (B_{3} + C_{3}z) \,_{3}F_{2}(a + 3, a2, a3; b_{1}, b_{2}; z) , (5.262)$

which has been found in Reference 49^2 with

$$B_1 = \frac{b_1b_2 + (a+1)(3a-2b_1-2b_2+4)}{(a-b_1+1)(a-b_2+1)}$$
 (5.263)

$$C_1 = \frac{(-a+a_2-1)(a-a_3+1)}{(a-b_1+1)(a-b_2+1)}$$
 (5.264)

$$B_2 = \frac{(a+1)(-3a+b_1+b_2-5)}{(a-b_1+1)(a-b_2+1)}$$
 (5.265)

$$C_2 = \frac{(a+1)(2a-a_2-a_3+3)}{(a-b_1+1)(a-b_2+1)}$$
(5.266)

$$B_3 = \frac{(a+1)(a+2)}{(a-b_1+1)(a-b_2+1)} \tag{5.267}$$

$$C_3 = -B_3.$$
 (5.268)

Using Eqs. (5.261) and (5.262) one arrives at the three-term recurrence relation

$$(n+2)(n+\ell/2-m+1)T_{mn+2}^{(\ell)} = \left[(\ell+3/2)(\ell/2-m) + (n+1) \times (3n+3\ell-2m+5) - (n+\ell/2+1)(n+\ell/2+5/2) \right] T_{mn+1}^{(\ell)} - (n+\ell/2-m)(n+\ell+3/2)T_{mn}^{(\ell)},$$
(5.269)

valid for $n \geq 0$ and provided that $m \neq n + \ell/2 + 1$, which represents also a recurrence relation for $\phi_{mn}^{(\ell)}$ [with quantities $\phi_{m0}^{(\ell)}$ and $\phi_{m1}^{(\ell)}$ shown in Eqs. (5.256) and (5.258)] since the proportionality factor does not depend on m [see Eq. (5.111)].

Similarly, Eq. (5.262) can be applied accordingly to Eq. (5.121) yielding, for $m \ge 2$ and $m \ne n + \ell/2$, the formula

$$2m(n + \ell/2 - m)T_{mn}^{(\ell)} = (n + 1 - 4m^2 + 4mn + 2m\ell + m - \ell^2/2)T_{m-1n}^{(\ell)} - (2m + 1)(n + \ell/2 + 1 - m)T_{m-2n}^{(\ell)},$$
 (5.270)

and, furthermore,

$$2m(n+\ell/2-m)\phi_{mn}^{(\ell)} = \frac{(n+1-4m^2+4mn+2m\ell+m-\ell^2/2)\sqrt{m}}{\sqrt{m+3/2}}\phi_{m-1n}^{(\ell)} - \frac{(2m+1)(n+\ell/2+1-m)\sqrt{m(m-1)}}{\sqrt{(m+1/2)(m+3/2)}}\phi_{m-2n}^{(\ell)},$$
 (5.271)

²http://functions.wolfram.com/07.27.17.0001.01

with $\phi_{0n}^{(\ell)}$ and $\phi_{1n}^{(\ell)}$ given by Eqs. (5.255) and (5.257), respectively.

5.6.6 Integral part

Next, one must calculate a recurrence relation for the quantity $U_{n\eta}^{(\ell)}$ defined in Eq. (5.92),

$$U_{n\eta}^{(\ell)} = \int_{0}^{\infty} dy y^{3} L_{n}^{(1/2)}(y^{2}/\gamma^{2}) e^{-y^{2}/\gamma^{2}} \frac{1}{2\eta} e^{-y^{2}} y^{\ell} L_{\eta-1}^{(\ell+1/2)}(y^{2}), \tag{5.272}$$

from which one arrives at the formula

$$(n+1) U_{n+1\eta}^{(\ell)} = \left[2n + 3/2 - \frac{1}{\gamma^2} (2\eta + \ell - 1/2) \right] U_{n\eta}^{(\ell)}$$

$$-(n+1/2) U_{n-1\eta}^{(\ell)} + \frac{1}{\gamma^2} \left[(\eta+1) U_{n\eta+1}^{(\ell)} + (\eta+\ell-1/2) \frac{(\eta-1)}{\eta} U_{n\eta-1}^{(\ell)} \right], \qquad (5.273)$$

valid for $n \ge 1$ and $\eta \ge 1$, and where again several identities of associated Laguerre polynomials have been utilized [47], namely

$$(n+1)L_{n+1}^{(\alpha)}(t) = (2n+\alpha+1-t)L_n^{(\alpha)}(t) - (n+\alpha)L_{n-1}^{(\alpha)}(t) (5.274)$$

$$tL_n^{(\alpha+1)}(t) = (n+\alpha+1)L_n^{(\alpha)}(t) - (n+1)L_{n+1}^{(\alpha)}(t) (5.275)$$

$$L_n^{(\alpha-1)}(t) = L_n^{(\alpha)}(t) - L_{n-1}^{(\alpha)}(t). \tag{5.276}$$

Here, Eq. (5.99) gives

$$U_{0\eta}^{(\ell)} = \frac{\Gamma(\ell/2+2)\Gamma(\eta+\ell+1/2)}{4\eta!\Gamma(\ell+3/2)} \frac{\gamma^{\ell+4}}{(1+\gamma^2)^{\ell/2+2}} \times F(1-\eta, \frac{\ell}{2}+2; \ell+\frac{3}{2}; \frac{\gamma^2}{1+\gamma^2}), \tag{5.277}$$

from which one obtains the equation

$$(\eta + 2) U_{0\eta+2}^{(\ell)} = -\frac{\eta(\eta + \ell + 1/2)}{(\eta + 1)(1 + \gamma^2)} U_{0\eta}^{(\ell)} + \left[2\eta + \ell + 3/2 - \frac{(\eta + \ell/2 + 2)\gamma^2}{(1 + \gamma^2)} \right] U_{0\eta+1}^{(\ell)}, (5.278)$$

where the Gauss' relation for contiguous hypergeometric functions (cf. Reference 47)

$$(c-a)F(a-1,b;c;z) = a(1-z)F(a+1,b;c;z) + [c-2a+(a-b)z]F(a,b;c;z), (5.279)$$

has been utilized. Due to $L_1^{1/2}(t) = 3/2 - t$, Eq. (5.272) can be rewritten as

$$U_{1\eta}^{(\ell)} = \frac{1}{2\eta} \int_{0}^{\infty} dy e^{-y^2(1+\gamma^{-2})} y^{\ell+3} \left(\frac{3}{2} - \frac{y^2}{\gamma^2}\right) L_{\eta-1}^{(\ell+1/2)}(y^2), \tag{5.280}$$

which, upon using Eqs. (5.275) and (5.276), yields for $\eta \geq 1$

$$\mathbf{U}_{1\eta}^{(\ell)} = \left[\frac{3}{2} - \frac{1}{\gamma^2} \left(2\eta + \ell - 1/2 \right) \right] \mathbf{U}_{0\eta}^{(\ell)} + \frac{1}{\gamma^2} \left[(\eta + 1) \mathbf{U}_{0\eta+1}^{(\ell)} + \frac{(\eta - 1)}{\eta} (\eta + \ell - 1/2) \mathbf{U}_{0\eta-1}^{(\ell)} \right].$$
(5.281)

The elements $U_{n0}^{(\ell)}$ may be evaluated by using Eq. (5.99),

$$U_{n0}^{(\ell)} = \frac{\gamma^{\ell+4}}{2(2\ell+1)(1+\gamma^2)^{\ell/2+2}} \sum_{k=0}^{n} \frac{(-1)^k}{k!} {n+1/2 \choose n-k} \times \frac{\Gamma(\ell/2+k+2)}{(1+\gamma^2)^k} F(1, \frac{\ell}{2}+k+2; \ell+\frac{3}{2}; \frac{\gamma^2}{1+\gamma^2}),$$
 (5.282)

together with several Gauss' relations for contiguous hypergeometric functions [47], namely

$$b(1-z)F(1,b+1;c;z) = c - 1 - (c-b-1)F(1,b;c;z),$$
(5.283)

and

$$F(1,b+1;c+2;z) = \frac{(c+1)}{(c-b)z} \left\{ 1 - \frac{c(1-z)}{bz} \left[F(1,b;c;z) - 1 \right] \right\}, \quad (5.284)$$

provided that $c \neq b$. The initial values with respect to F are given by

$$F(1,2;\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) = \frac{(1+\gamma^2)}{2} \left[1 + \frac{(1+\gamma^2)}{\gamma} \arctan \gamma \right], \qquad (5.285)$$

as well as

$$F(1, \frac{7}{2}; \frac{9}{2}; \frac{\gamma^2}{1+\gamma^2}) = \frac{7(1+\gamma^2)^{7/2}}{\gamma^7} \ln\left(\gamma + \sqrt{1+\gamma^2}\right) - \frac{7(1+\gamma^2)^2(3+4\gamma^2)}{3\gamma^6} - \frac{7(1+\gamma^2)}{5\gamma^2}.$$
 (5.286)

Recalling Eq. (5.272),

$$U_{n\eta}^{(\ell+2)} = \frac{1}{2\eta} \int_{0}^{\infty} dy e^{-y^2(1+\gamma^{-2})} L_n^{(1/2)}(y^2/\gamma^2) y^{\ell+3} y^2 L_{\eta-1}^{(\ell+5/2)}(y^2), \qquad (5.287)$$

a recurrence identity regarding the parameter ℓ may be obtained, yielding for $\eta \geq 1$

$$U_{n\eta}^{(\ell+2)} = \frac{(\ell+3/2)}{\eta} \sum_{j=0}^{\eta-1} (j+1) U_{nj+1}^{(\ell)} - (\eta+1) U_{n\eta+1}^{(\ell)}, \tag{5.288}$$

where Eq. (5.275) and the relationship [29]

$$L_n^{(\alpha+1)}(x) = \sum_{j=0}^n L_j^{(\alpha)}(x)$$
 (5.289)

have been used. From Eq. (5.288), by shifting $\eta \to \eta + 1$, one gets for $\eta \ge 0$ the result

$$U_{n\eta+1}^{(\ell+2)} = \frac{\eta}{(\eta+1)} U_{n\eta}^{(\ell+2)} + (\eta+\ell+3/2) U_{n\eta+1}^{(\ell)} - (\eta+2) U_{n\eta+2}^{(\ell)}.$$
 (5.290)

In virtue of Eq. (5.277) with $\eta=0$ and after applying Eq. (5.284) it follows that

$$U_{00}^{(\ell+2)} = \frac{\Gamma(\ell/2+2)}{4(\ell-1)} \frac{\gamma^{\ell+2}}{(1+\gamma^2)^{\ell/2+2}} \left[(\ell+4)\gamma^2 + 2\ell + 3 \right] - \frac{(2\ell+1)(2\ell+3)}{2(\ell-1)\gamma^2} U_{00}^{(\ell)},$$
(5.291)

valid for $\ell \neq 1$. Since F(0,b;c;z) = 1, one obtains from Eq. (5.99) the expression

$$U_{n1}^{(\ell)} = \binom{n+1/2}{n} \frac{\Gamma(\ell/2+2)}{4} \frac{\gamma^{\ell+4}}{(1+\gamma^2)^{\ell/2+2}} F(-n, \frac{\ell}{2}+2; \frac{3}{2}; \frac{1}{1+\gamma^2}), \quad (5.292)$$

which has been calculated by means of MAPLE [48]. From this relationship it immediately follows that

$$U_{01}^{(\ell)} = \frac{\Gamma(\ell/2+2)}{4} \frac{\gamma^{\ell+4}}{(1+\gamma^2)^{\ell/2+2}},$$
 (5.293)

and, furthermore,

$$U_{01}^{(\ell+2)} = \frac{(\ell+4)}{2} \frac{\gamma^2}{(1+\gamma^2)} U_{01}^{(\ell)}.$$
 (5.294)

The initial value for $\ell = 0$ reads

$$U_{00}^{(0)} = \frac{\gamma^4}{2(1+\gamma^2)^2} F(1,2;\frac{3}{2};\frac{\gamma^2}{1+\gamma^2})$$

$$= \frac{\gamma^3}{4} \left[\frac{\gamma}{(1+\gamma^2)} + \arctan \gamma \right], \qquad (5.295)$$

where Eqs. (5.277) and (5.285) have been employed whereas Eqs. (5.277) and (5.286) add up to the initial value for $\ell = 3$

$$U_{00}^{(3)} = \frac{15\sqrt{\pi}}{16} \left[\ln\left(\gamma + \sqrt{1+\gamma^2}\right) - \frac{\gamma(3+4\gamma^2)}{3(1+\gamma^2)^{3/2}} - \frac{\gamma^5}{5(1+\gamma^2)^{5/2}} \right]. \quad (5.296)$$

One may derive corresponding recurrence relations for the special cases $\ell=0$ and $\ell=1$, respectively, by revisiting Eqs. (5.100) and (5.108). Here, Eq. (5.100) yields the identity

$$(n+2) U_{n+2\eta}^{(0)} = -\frac{(n+\eta)(n+3/2)}{(n+1)} \frac{\gamma^2}{(1+\gamma^2)} U_{n\eta}^{(0)} + \left[2n+\eta+5/2 - \frac{(n+\eta+2)}{(1+\gamma^2)} \right] U_{n+1\eta}^{(0)}, \quad (5.297)$$

where again Eq. (5.279) has been applied and where $U_{0\eta}^{(0)}$ and $U_{1\eta}^{(0)}$ follow from Eqs. (5.278) and (5.281). The initial value $U_{10}^{(0)}$ has to be calculated by using Eq. (5.100) yielding

$$U_{10}^{(0)} = -\frac{\gamma^4}{4(1+\gamma^2)^2}. (5.298)$$

The simplest way to derive a recursion for $U_{n\eta}^{(1)}$ is to employ first Eq. (5.108) yielding

$$U_{n\eta}^{(1)} = \frac{\Gamma(n+\eta+1/2)\gamma^{2n+3}}{4n!\eta!(1+\gamma^2)^{n+\eta+1/2}} \left[\eta+1/2 - \frac{(n+\eta+1/2)}{(1+\gamma^2)}\right]$$
(5.299)

$$= \frac{(\eta+1/2)\Gamma(n+\eta+1/2)\gamma^{2n+3}}{4n!\eta!(1+\gamma^2)^{n+\eta+1/2}}F(-1,n+\eta+\frac{1}{2};\eta+\frac{1}{2};\frac{1}{1+\gamma^2}), (5.300)$$

where F(-1, b; c; z) = 1 - bz/c has been applied [47], and then to use the equation

$$b(1-z)F(-1,b+1;c;z) = (c-b)F(-1,b-1;c;z) + [2b-c-(b+1)z]F(-1,b;c;z), (5.301)$$

producing the following the three-term recurrence relation

$$(n+2) U_{n+2\eta}^{(1)} = -(n+\eta+1/2) \frac{\gamma^2}{(1+\gamma^2)} U_{n\eta}^{(1)} + \left[2n+\eta+5/2 - \frac{(n+\eta+5/2)}{(1+\gamma^2)} \right] U_{n+1\eta}^{(1)}. (5.302)$$

The recursions for $U_{0\eta}^{(1)}$ and $U_{1\eta}^{(1)}$ follow immediately from Eqs. (5.299) and (5.300), respectively,

$$U_{0\eta+1}^{(1)} = \frac{(\eta + 3/2)}{(\eta + 1)(1 + \gamma^2)} U_{0\eta}^{(1)}$$
(5.303)

$$U_{1\eta}^{(1)} = \left[(\eta + 3/2) \frac{\gamma^2}{(1+\gamma^2)} - 1 \right] U_{0\eta}^{(1)}, \tag{5.304}$$

where the initial value is given by

$$U_{00}^{(1)} = \frac{\sqrt{\pi}}{8} \frac{\gamma^5}{(1+\gamma^2)^{3/2}}.$$
 (5.305)

In Section 5.3.1 [see Eq. (5.71)] the matrix elements of the field particle operator in terms of φ_m test function basis were found to be

$$I_{mm'}^{(\ell)} = \sum_{n=0}^{m} \sum_{n'=0}^{N'} \frac{2}{h_n^{(0)} h_{n'}^{(\ell)}} \phi_{mn}^{(0)} \hat{I}_{nn'}^{(\ell)} \phi_{n'm'}^{(\ell)}, \tag{5.306}$$

which, for numerical reasons, is rewritten in the form

$$I_{mm'}^{(\ell)} = \sum_{n=0}^{m} \sum_{n'=0}^{N'} \left(\frac{2\phi_{mn}^{(0)}}{h_n^{(0)}}\right) \left(\frac{\hat{I}_{nn'}^{(\ell)}}{\sqrt{h_{n'}^{(\ell)}}}\right) \left(\frac{\phi_{n'm'}^{(\ell)}}{\sqrt{h_{n'}^{(\ell)}}}\right)$$

$$\equiv \sum_{n=0}^{m} \sum_{n'=0}^{N'} g_{mn}^{(0)} \, \hat{G}_{nn'}^{(\ell)} \, \hat{g}_{n'm'}^{(\ell)}. \tag{5.307}$$

With this definition values of the normalized matrices in the last equation are approximately $\mathcal{O}(1)$ or less minimizing difficulties appearing during the numerical evaluation of matrix elements, e.g., loss of significance due to subtractive cancellation.

The normalizing factor $h_n^{(\ell)}$ has been defined by

$$h_n^{(\ell)} = \frac{1}{(2\ell+1)} \frac{\Gamma(n+\ell+3/2)}{\pi^{3/2} n!},\tag{5.308}$$

from which one easily finds the relations

$$h_{n+1}^{(\ell)} = \frac{(n+\ell+3/2)}{(n+1)} h_n^{(\ell)}, \tag{5.309}$$

and

$$h_n^{(\ell+1)} = \frac{(2\ell+1)}{(2\ell+3)} (n+\ell+3/2) h_n^{(\ell)}.$$
 (5.310)

Recalling the definition of transformation matrix, $\phi_{mn}^{(\ell)} \equiv T_{mn}^{(\ell)}/(\pi^{3/4}\sqrt{h_m})$, it follows from Eqs. (5.116) and (5.308) that

$$g_{mn}^{(0)} = \begin{cases} \pi^{3/4} \sqrt{\frac{2m!}{\Gamma(m+5/2)}} & \text{for } n \le m \\ 0 & \text{for } n > m, \end{cases}$$
 (5.311)

where $h_m = \Gamma(m + 5/2)/(2m!)$ has been used. This leads immediately to the recursion

$$g_{m+10}^{(0)} = \sqrt{\frac{(m+1)}{(m+5/2)}} g_{m0}^{(0)}, \tag{5.312}$$

with the initial value

$$g_{00}^{(0)} = 2\sqrt{\frac{2\pi}{3}}. (5.313)$$

The respective recurrence relation for the quantity $\hat{g}_{mn}^{(\ell)}$ is obtained from Eq. (5.252),

$$\sqrt{(m+1)(m+5/2)}\hat{g}_{m+1n}^{(\ell)} = -\sqrt{m(m+3/2)}\hat{g}_{m-1n}^{(\ell)}
+ (2m-2n-\ell+1)\hat{g}_{mn}^{(\ell)} + \sqrt{n(n+\ell+1/2)}\hat{g}_{mn-1}^{(\ell)}
+ \sqrt{(n+1)(n+\ell+3/2)}\hat{g}_{mn+1}^{(\ell)},$$
(5.314)

where again Eq. (5.309) has been used (note that $\hat{g}_{mn}^{(\ell)} = \hat{g}_{nm}^{(\ell)}$).

The recursions derived from a recurrence identity for the generalized hypergeometric function ${}_{3}F_{2}(a,b,c;d,e;z)$ become [see Eqs. (5.269) and (5.271) in Section 5.6.5]

$$(n+\ell/2-m)\sqrt{(n+1)(n+\ell+3/2)}\hat{g}_{mn+1}^{(\ell)} = \left[(\ell+3/2)(\ell/2-m) + n(3n+3\ell-2m+2) - (n+\ell/2)(n+\ell/2+3/2) \right] \hat{g}_{mn}^{(\ell)} - (n+\ell/2-m-1)\sqrt{n(n+\ell+1/2)}\hat{g}_{mn-1}^{(\ell)}, \quad (5.315)$$

and

$$2m(n + \ell/2 - m)\hat{g}_{mn}^{(\ell)} = \frac{(n + 1 - 4m^2 + 4mn + 2m\ell + m - \ell^2/2)\sqrt{m}}{\sqrt{m + 3/2}}\hat{g}_{m-1n}^{(\ell)} - \frac{(2m + 1)(n + \ell/2 + 1 - m)\sqrt{m(m - 1)}}{\sqrt{(m + 1/2)(m + 3/2)}}\hat{g}_{m-2n}^{(\ell)},$$
 (5.316)

respectively. By means of Eqs. (5.254)-(5.260) along with Eqs. (5.309) and (5.310) one arrives at the following identities,

$$\hat{g}_{0n+1}^{(\ell)} = \frac{(n+\ell/2)}{\sqrt{(n+1)(n+\ell+3/2)}} \hat{g}_{0n}^{(\ell)}$$
 (5.317)

$$\hat{g}_{m+10}^{(\ell)} = \frac{(m-\ell/2+1)}{\sqrt{(m+1)(m+5/2)}} \hat{g}_{m0}^{(\ell)}, \tag{5.318}$$

and

$$\hat{g}_{1n+1}^{(\ell)} = \frac{\left[5(2n+\ell) - (\ell+3)(\ell-2)\right]}{2\sqrt{5(n+1)(2n+2\ell+3)}} \,\hat{g}_{0n}^{(\ell)} \tag{5.319}$$

$$\hat{g}_{m+11}^{(\ell)} = \frac{(2\ell+3)(2m+2-\ell) + \ell(\ell+3)}{4\sqrt{(m+1)(m+5/2)(\ell+3/2)}} \,\hat{g}_{m0}^{(\ell)}, \tag{5.320}$$

as well as

$$\sqrt{n+\ell+7/2}\hat{g}_{mn+1}^{(\ell+2)} = \sqrt{n+1}\hat{g}_{mn}^{(\ell+2)} + \sqrt{\frac{2\ell+5}{2\ell+1}} \times \left(\sqrt{n+\ell+5/2}\hat{g}_{mn+1}^{(\ell)} - \sqrt{n+2}\hat{g}_{mn+2}^{(\ell)}\right). (5.321)$$

The initial values

$$\hat{g}_{00}^{(0)} = \frac{1}{\sqrt{3}}, \qquad \hat{g}_{00}^{(1)} = 2\sqrt{\frac{2}{3\pi}},$$
 (5.322)

have been computed using the relation

$$\hat{g}_{00}^{(\ell)} = \frac{\Gamma(\ell/2 + 3/2)}{\pi^{1/4}} \sqrt{\frac{2(2\ell + 1)}{3\Gamma(\ell + 3/2)}},$$
(5.323)

from which one infers that

$$\hat{g}_{00}^{(\ell+2)} = \frac{(\ell+3)}{\sqrt{(2\ell+1)(2\ell+3)}} \hat{g}_{00}^{(\ell)}.$$
 (5.324)

The normalized matrix elements in the Burnett function basis, $\hat{G}_{nn'}^{(\ell)}$, can now be calculated by means of the above presented recurrence identities regarding the quantity $U_{n\eta}^{(\ell)}$. Therefore, details of the calculations of the necessary recursions are not given here, only the final forms of results are presented.

Upon introducing the quantity $\hat{\mathbf{U}}_{n\eta}^{(\ell)} \equiv \mathbf{U}_{n\eta}^{(\ell)}/[h_{\eta}^{(\ell)}]^{1/2}$ the representation of matrix elements in terms of Burnett functions [see Eq. (5.91)] may be rewritten in the form

$$\hat{G}_{nn'}^{(\ell)} = \frac{3(2n'+\ell)}{\pi^{3/2}\gamma^5} \left[(1+\gamma^2) \, \hat{\mathbf{U}}_{nn'}^{(\ell)} - \frac{(2n'+\ell-1)}{\sqrt{2n'(2n'+2\ell+1)}} \, \hat{\mathbf{U}}_{nn'-1}^{(\ell)} \right], \quad (5.325)$$

valid for $n' \ge 1$, where Eqs. (5.307) and (5.309) have been used. The matrix elements $\hat{G}_{n0}^{(\ell)}$ may be evaluated according to Eq. (5.101),

$$\hat{G}_{n0}^{(\ell)} \equiv \frac{\hat{I}_{n0}^{(\ell)}}{\sqrt{h_0^{(\ell)}}} = \left[\frac{2\pi^{3/2}}{\Gamma(\ell+1/2)} \right]^{1/2} \hat{I}_{n0}^{(\ell)}, \tag{5.326}$$

yielding

$$\hat{G}_{n0}^{(\ell)}(\gamma_{ab}) = \frac{3\ell}{\pi^{3/4}(2\ell+1)\sqrt{2\Gamma(\ell+1/2)}} \frac{\gamma_{ab}^{\ell-1}}{(1+\gamma_{ab}^2)^{\ell/2+1}} \times \sum_{k=0}^{n} \frac{(-1)^k}{k!} \binom{n+1/2}{n-k} \frac{\Gamma(\ell/2+k+2)}{(1+\gamma_{ab}^2)^k} \mathcal{P}_0^{(\ell)}(k,\gamma_{ab}), \quad (5.327)$$

with

$$P_0^{(\ell)}(k,\gamma) = F(1, \frac{\ell}{2} + k + 2; \ell + \frac{3}{2}; \frac{\gamma^2}{1+\gamma^2}) - \frac{(\ell-1)}{(2\ell-1)(1+\gamma^2)} F(2, \frac{\ell}{2} + k + 2; \ell + \frac{3}{2}; \frac{\gamma^2}{1+\gamma^2}),$$
 (5.328)

noticing that $\hat{G}_{n0}^{(0)} = 0$. The computation of the Gauss series is carried out with the help of Eqs. (5.283)-(5.286) and, additionally, by applying the relation (cf. Reference 47)

$$(1-z)F(2,b;c;z) = c - 1 + [2 - c + (b-1)z]F(1,b;c;z).$$
 (5.329)

Due to the fact that the normalizing factor, $h_{n'}^{(\ell)}$, does not depend on index n the above obtained recurrence relations with respect to n for the quantity $U_{n\eta}^{(\ell)}$ can be used unchanged. All other relations must be adjusted in virtue

of Eqs. (5.309) and (5.310) noting that one needs to adapt the initial values accordingly. The corresponding modified recurrence identities become

$$(n+1) \hat{\mathbf{U}}_{n+1\eta}^{(\ell)} = \left[2n + 3/2 - \frac{1}{\gamma^2} (2\eta + \ell - 1/2) \right] \hat{\mathbf{U}}_{n\eta}^{(\ell)}$$

$$- (n+1/2) \hat{\mathbf{U}}_{n-1\eta}^{(\ell)} + \frac{1}{\gamma^2} \left[\frac{(\eta + \ell - 1/2)(\eta - 1)}{\sqrt{\eta(\eta + \ell + 1/2)}} \hat{\mathbf{U}}_{n\eta - 1}^{(\ell)} + \sqrt{(\eta + 1)(\eta + \ell + 3/2)} \hat{\mathbf{U}}_{n\eta + 1}^{(\ell)} \right],$$

$$(5.330)$$

$$\hat{\mathbf{U}}_{0\eta+2}^{(\ell)} = -\frac{\eta(\eta + \ell + 1/2)}{\sqrt{(\eta+1)(\eta+2)(\eta+\ell+3/2)(\eta+\ell+5/2)}} \frac{\hat{\mathbf{U}}_{0\eta}^{(\ell)}}{(1+\gamma^2)}
+ \left[2\eta + \ell + 3/2 - \frac{(\eta+\ell/2+2)\gamma^2}{(1+\gamma^2)} \right] \frac{\hat{\mathbf{U}}_{0\eta+1}^{(\ell)}}{\sqrt{(\eta+2)(\eta+\ell+5/2)}}, \quad (5.331)$$

$$\hat{\mathbf{U}}_{1\eta}^{(\ell)} = \frac{1}{\gamma^2} \left[\sqrt{(\eta+1)(\eta+\ell+3/2)} \, \hat{\mathbf{U}}_{0\eta+1}^{(\ell)} + \frac{(\eta-1)(\eta+\ell-1/2)}{\sqrt{\eta(\eta+\ell+1/2)}} \, \hat{\mathbf{U}}_{0\eta-1}^{(\ell)} \right] \\
+ \left[\frac{3}{2} - \frac{1}{\gamma^2} (2\eta+\ell-1/2) \right] \, \hat{\mathbf{U}}_{0\eta}^{(\ell)}.$$
(5.332)

The recursions involving the parameter ℓ have the form

$$\sqrt{\eta + \ell + 7/2} \,\,\hat{\mathbf{U}}_{n\eta+1}^{(\ell+2)} = \frac{\eta}{\sqrt{\eta + 1}} \,\,\hat{\mathbf{U}}_{n\eta}^{(\ell+2)} + \sqrt{\frac{2\ell + 5}{2\ell + 1}} \\
\times \,\,\left[\frac{(\eta + \ell + 3/2)}{\sqrt{\eta + \ell + 5/2}} \,\,\hat{\mathbf{U}}_{n\eta+1}^{(\ell)} - \sqrt{\eta + 2} \,\,\hat{\mathbf{U}}_{n\eta+2}^{(\ell)} \right], (5.333)$$

$$(\ell - 1) \hat{\mathbf{U}}_{00}^{(\ell+2)} = \frac{\pi^{3/4} \Gamma(\ell/2 + 3)}{\sqrt{2\Gamma(\ell + 5/2)}} \frac{\gamma^{\ell+2}}{(1 + \gamma^2)^{\ell/2+2}} \left[\gamma^2 + \frac{(2\ell + 3)}{(\ell + 4)} \right] - \frac{2}{\gamma^2} \sqrt{(\ell + 1/2)(\ell + 3/2)} \, \hat{\mathbf{U}}_{00}^{(\ell)}, \tag{5.334}$$

and

$$\sqrt{(\ell+1/2)(\ell+7/2)} \,\,\hat{\mathbf{U}}_{01}^{(\ell+2)} = (\ell/2+2) \,\frac{\gamma^2}{(1+\gamma^2)} \,\,\hat{\mathbf{U}}_{01}^{(\ell)}. \tag{5.335}$$

If the index $\ell = 0$ and $\ell = 1$ the respective relations read

$$(n+2)\hat{\mathbf{U}}_{n+2\eta}^{(0)} = -\frac{(n+\eta)(n+3/2)}{(n+1)} \frac{\gamma^2}{(1+\gamma^2)} \hat{\mathbf{U}}_{n\eta}^{(0)} + \left[2n+\eta+5/2 - \frac{(n+\eta+2)}{(1+\gamma^2)}\right] \hat{\mathbf{U}}_{n+1\eta}^{(0)}$$
(5.336)

$$(n+2)\hat{\mathbf{U}}_{n+2\eta}^{(1)} = -(n+\eta+1/2) \frac{\gamma^2}{(1+\gamma^2)} \hat{\mathbf{U}}_{n\eta}^{(1)} + \left[2n+\eta+5/2 - \frac{(n+\eta+5/2)}{(1+\gamma^2)}\right] \hat{\mathbf{U}}_{n+1\eta}^{(1)},$$
(5.337)

with

$$\hat{\mathbf{U}}_{0\eta+1}^{(1)} = \frac{(\eta+3/2)}{\sqrt{(\eta+1)(\eta+5/2)}(1+\gamma^2)} \,\hat{\mathbf{U}}_{0\eta}^{(1)} \tag{5.338}$$

$$\hat{\mathbf{U}}_{1\eta}^{(1)} = \left[(\eta + 3/2) \frac{\gamma^2}{(1+\gamma^2)} - 1 \right] \hat{\mathbf{U}}_{0\eta}^{(1)}. \tag{5.339}$$

Finally, the normalized initial values are given by

$$\hat{\mathbf{U}}_{00}^{(0)} = \sqrt{2\pi} \frac{\gamma^3}{4} \left[\frac{\gamma}{(1+\gamma^2)} + \arctan \gamma \right]$$
 (5.340)

$$\hat{\mathbf{U}}_{00}^{(1)} = \frac{\pi}{4} \frac{\gamma^5}{(1+\gamma^2)^{3/2}} \tag{5.341}$$

$$\hat{\mathbf{U}}_{00}^{(3)} = \frac{\sqrt{15}\pi}{4} \left[\ln(\gamma + \sqrt{1+\gamma^2}) - \frac{\gamma(3+4\gamma^2)}{3(1+\gamma^2)^{3/2}} - \frac{\gamma^5}{5(1+\gamma^2)^{5/2}} \right], (5.342)$$

as well as

$$\hat{\mathbf{U}}_{01}^{(0)} = \frac{\pi^{1/2}}{2\sqrt{3}} \frac{\gamma^4}{(1+\gamma^2)^2} \tag{5.343}$$

$$\hat{\mathbf{U}}_{01}^{(1)} = \frac{3\pi}{4\sqrt{10}} \frac{\gamma^5}{(1+\gamma^2)^{5/2}},\tag{5.344}$$

and

$$\hat{\mathbf{U}}_{10}^{(0)} = -\frac{\sqrt{2\pi}}{4} \frac{\gamma^4}{(1+\gamma^2)^2}.$$
 (5.345)

Furthermore, the elements $\hat{\mathbf{U}}_{n0}^{(\ell)}$ are evaluated by means of Eqs. (5.282)-(5.286) and Eq. (5.308), respectively.

According to Eq. (5.307) the recurrence relation for the matrix elements of the field particle operator in terms of φ_m test functions is found to be

$$I_{m+1m'}^{(\ell)} = \sum_{n=0}^{m+1} \sum_{n'=0}^{N'} g_{m+1n}^{(0)} \, \hat{G}_{nn'}^{(\ell)} \, \hat{g}_{n'm'}^{(\ell)}$$

$$= \sqrt{\frac{m+1}{m+5/2}} I_{mm'}^{(\ell)} + g_{m+10}^{(0)} \sum_{n'=0}^{N'} \hat{G}_{m+1n'}^{(\ell)} \, \hat{g}_{n'm'}^{(\ell)}, \qquad (5.346)$$

where Eqs. (5.311) and (5.312) have been utilized.

5.6.7 Numerical implementation

In a concluding section the numerical implementation of the calculation of collision matrix elements is briefly considered. First of all, it should be mentioned that most of the analytical results obtained in Chapter 5 were checked and partially derived, respectively, by means of the symbolic algebra system MAPLE [48]. Due to the fact that the computing time required to evaluate the matrix elements regarding the field particle operator became too large using MAPLE the actual calculation of them, however, was performed using FORTRAN90.

Since in neoclassical transport theory the expansion of the distribution function in terms of associated Laguerre polynomials [cf. test functions φ_m in Eq. (5.2)] tends to converge quickly [22,37] only a small number of terms (indicated by the radial index m) have to be retained in the expansion. For the numerical computation m_{max} and m'_{max} were chosen to be 10.

Therefore, computing of the matrix elements of the test particle operator, $\hat{\nu}_{mm'}^{ab}$ and $\hat{D}_{mm'}^{ab}$, respectively, by using their recurrence relations [see Eqs. (5.188), (5.220) and (5.230)] is possible without any difficulty with respect to numerical accuracy.

Unfortunately, this is not valid for the matrix elements describing the field particle operator, $I_{mm'}^{(\ell)}$ [see Eq. (5.346)]. Because these elements have been obtained via transformation from the Burnett function basis an additional summation (over index n', with N' as large as possible) must be performed producing a large numerical error for the case when conventional double precision FORTRAN90 is used. Thus, in order to decrease round-off errors a FORTRAN90 based multiple precision computation package, MPFUN90, developed by D. H. Bailey [50–53] has been utilized. By means of these routines the value of the parameter N' (which is the only parameter determining the accuracy of the matrix elements $I_{mm'}^{(\ell)}$) could be chosen to be 6×10^6 , which allowed to obtain highly accurate results for the matrix elements $I_{mm'}^{(\ell)}$. They

are correct to at least five (for larger values of ℓ , m and m') to eight (for smaller values of ℓ , m and m') significant digits. In order to ensure that the calculations provided numerically converged values (no round-off computational errors) the code was run twice, namely using precision levels of 200 and 300 digits, respectively.

Altogether the computing time for the matrices $\hat{\nu}_{mm'}^{ee}$, $\hat{\nu}_{mm'}^{e\infty}$ and $\hat{D}_{mm'}^{ee}$ was less than one second (for $m_{max} = m'_{max} = 10$), whereas for an individual element with respect to the electron-electron version of the field particle part $I_{mm'}^{(\ell)}$ (polar index $\ell_{max} = 20$) average time of calculation was typically of the order of 100 seconds (for $N' = 6 \times 10^6$). All computations were performed on an Intel Core2Duo CPU (E8500) 3.16GHz and 3GB RAM running Linux (2.6.32-trunk-686).

Chapter 6

Spitzer conductivity

Below, the formulas derived in Chapter 3 together with the collision matrix elements evaluated in Chapter 5 are used to compute the collisional Spitzer (or classical) conductivity for a completely ionized gas. Since the correct result is only obtained when the full linearized Coulomb collision operator is applied, this problem serves as a benchmark for the matrix elements.

Cohen et al. [45] as well as Spitzer and Härm [39] calculated in their classical papers the parallel electrical (DC-) conductivity for a uniform plasma when no magnetic field is present and where a sufficiently small electric field is assumed (see also References 54–57). In Reference 39 the following expression for the conductivity was obtained

$$\sigma = \frac{2mC^3}{e^2 Z \ln(qC^2)} \left(\frac{2}{3\pi}\right)^{3/2} \gamma_E , \qquad (6.1)$$

where γ_E is the ratio of conductivity to that in a Lorentz gas. Here, C is the root mean square electron velocity $C = \sqrt{3T_e/m_e} = v_{te}\sqrt{3/2}$, $v_{te} = \sqrt{2T_e/m_e}$ and $\ln(qC^2)$ designates the Coulomb logarithm. In terms of the notation used in previous chapters Eq. (6.1) can be rewritten as

$$\sigma = \frac{2m_e v_{te}^3}{\pi^{3/2} e^2 Z_{\text{eff}} \ln \Lambda} \gamma_E. \tag{6.2}$$

In order to obtain the Spitzer conductivity within the NEO-2 model one has to assume a homogeneous magnetic field (that is, the magnetic field module \hat{B} does not depend on s being the distance counted along the magnetic field line).

From Eqs. (3.40) and (3.42) one gets for the electric current density in response to the induced parallel electric field,

$$\langle j_{\parallel} \rangle = eL_{33}^{e}A_{3}$$

$$= -eL_{33}^{e}\frac{e}{T_{e}}\langle E_{\parallel}^{(A)} \rangle, \qquad (6.3)$$

in which the forces A_1 and A_2 have been put to zero. The parallel electric conductivity is then defined as

$$\sigma_{\parallel}^{\text{NEO}} \equiv \frac{\langle j_{\parallel} \rangle}{\langle E_{\parallel}^{(A)} \rangle}.$$
 (6.4)

Upon substituting the transport coefficient $L_{33}^e = n_e l_c^2 \gamma_{33} / \tau_{ee}$ into Eq. (6.3) one obtains from Eq. (6.4)

$$\sigma_{\parallel}^{\text{NEO}} = -\frac{n_e}{\tau_{ee}} l_c^2 \gamma_{33} \frac{e^2}{T_e} \tag{6.5}$$

$$= -\frac{2n_e e^2 \tau_{ee}}{m_e} \gamma_{33}$$

$$= -\frac{3m_e v_{te}^3}{8\sqrt{\pi}e^2 \ln \Lambda} \gamma_{33}.$$
(6.6)

$$= -\frac{3m_e v_{te}^3}{8\sqrt{\pi}e^2 \ln \Lambda} \gamma_{33}. \tag{6.7}$$

From Eqs. (6.2) and (6.7) the relation between the normalized Spitzer conductivity and the dimensionless NEO-2 transport coefficient γ_{33} can be expressed as

$$\gamma_E = -\frac{3\pi Z_{\text{eff}}}{16} \gamma_{33}. \tag{6.8}$$

6.1 Lorentz conductivity

The electrical conductivity can be calculated analytically for the case when the limit $Z_{\text{eff}} \to \infty$ is assumed (the so called "Lorentz gas approximation"). In such a fully ionized plasma the electrons do not interact with each other and all the positive ions are at rest [54].

The single-drive problem [see Chapter 3, Eq. (3.22)] for the evaluation of the parallel conductivity can be written as

$$C_e^l[f_3^{\sigma}] = f_{e0}Q_3^{-\sigma} , \qquad (6.9)$$

where the collision term is approximated by a Lorentz operator

$$C_e^l \equiv \mathcal{L} = \frac{\nu_D^e}{2} \frac{\partial}{\partial \lambda} \left(1 - \lambda^2 \right) \frac{\partial}{\partial \lambda}.$$
 (6.10)

Equations of the form (6.9) are called Spitzer problems [23]. Assuming stationary ions the deflection frequency here means [cf. Eqs. (3.75) and (3.78)],

$$\nu_D^e = Z_{\text{eff}} \frac{3\sqrt{\pi}}{4\tau_{ee}} \left(\frac{v_{te}}{v}\right)^3, \tag{6.11}$$

keeping in mind that electron-electron collisions have been ignored and where $Q_3^{\sigma} = v|\lambda|q_3^{\sigma}$ and $q_3^{\sigma} = \sigma \hat{B}$, respectively. With the help of the normalization

$$f_3^{\sigma} = f_{e0} f_{sp}^L, \tag{6.12}$$

where the subscript L refers to the Lorentz approximation one gets

$$\frac{\nu_D^e}{2} \frac{\partial}{\partial \lambda} \left(1 - \lambda^2 \right) \frac{\partial}{\partial \lambda} f_{sp}^L = -v \lambda \hat{B}. \tag{6.13}$$

where $\hat{B} = 1$ has been used. One can solve Eq. (6.13) for the Spitzer function by applying the Legendre polynomial, P_{ℓ} , expansion, that is

$$f_{sp}^{L} = \sum_{\ell} c_{\ell}(v) P_{\ell}(\lambda). \tag{6.14}$$

Since these polynomials are eigenfunctions of the Lorentz collision operator [58],

$$\frac{\partial}{\partial \lambda} \left(1 - \lambda^2 \right) \frac{\partial}{\partial \lambda} P_{\ell}(\lambda) = -\ell(\ell+1) P_{\ell}(\lambda), \tag{6.15}$$

it follows from Eqs. (6.13)-(6.15) that

$$\frac{\nu_D^e}{2} \frac{\partial}{\partial \lambda} \left(1 - \lambda^2 \right) \frac{\partial}{\partial \lambda} \left[\sum_{\ell} c_{\ell}(v) P_{\ell}(\lambda) \right] = -v P_1(\lambda) \hat{B}$$

$$- \frac{\nu_D^e}{2} \sum_{\ell} c_{\ell}(v) \ell(\ell+1) P_{\ell}(\lambda) = -v P_1(\lambda) \hat{B}. \tag{6.16}$$

Upon multiplication of Eq. (6.16) by $P_{\ell'}$, integrating the result with respect to λ from -1 to 1 and exploiting the orthogonality of Legendre polynomials [29],

$$\int_{-1}^{1} d\lambda P_{\ell}(\lambda) P_{\ell'}(\lambda) = \frac{2}{2\ell + 1} \delta_{\ell\ell'}, \tag{6.17}$$

one easily recognizes the only nonvanishing coefficient

$$c_1 = \frac{\hat{B}}{\kappa^{\text{mono}}}. (6.18)$$

Here, the abbreviation $\kappa^{\text{mono}}(v) \equiv \nu_D(v)/v$ has been introduced. Therefore, the normalized Spitzer function becomes

$$f_{sp}^{L} = \frac{\lambda \hat{B}}{\kappa^{\text{mono}}}.$$
 (6.19)

Using Eq. (3.63) one finds in the Lorentz limit for the monoenergetic transport coefficient describing electric conductivity of a plasma along the magnetic field, D_{33} ,

$$D_{33}^{L} = v_{te} \beta_3^2 x \sum_{\sigma = \pm 1} \left\langle \frac{\hat{B}}{4} \int_{0}^{1/\hat{B}} d\eta q_3^{-\sigma} f_{sp}^L \right\rangle.$$
 (6.20)

Since

$$\sum_{\sigma=\pm 1} \left\langle \frac{\hat{B}}{4} \int_{0}^{1/\hat{B}} d\eta \frac{1}{|\lambda|} A^{\sigma}(\eta) \right\rangle = \left\langle \frac{1}{2} \int_{-1}^{1} d\lambda A(\lambda) \right\rangle , \qquad (6.21)$$

Eq. (6.20) becomes

$$D_{33}^{L} = -v \sum_{\sigma=\pm 1} \left\langle \frac{\hat{B}}{4} \int_{0}^{1/\hat{B}} d\eta q_{3}^{\sigma} f_{sp}^{L} \right\rangle$$

$$= -v \sum_{\sigma=\pm 1} \left\langle \frac{\hat{B}}{4} \int_{0}^{1/\hat{B}} d\eta \frac{1}{|\lambda|} |\lambda| \sigma \hat{B} f_{sp}^{L} \right\rangle$$

$$= -v \left\langle \frac{1}{2} \int_{-1}^{1} d\lambda \lambda \hat{B} f_{sp}^{L} \right\rangle$$

$$= -v \frac{\langle \hat{B}^{2} \rangle}{\kappa^{\text{mono}}} \frac{1}{2} \int_{-1}^{1} d\lambda \lambda^{2}$$

$$= -\frac{v \langle \hat{B}^{2} \rangle}{3\kappa^{\text{mono}}}, \qquad (6.22)$$

where Eq. (6.19) has been utilized (note that here $\langle \hat{B}^2 \rangle = \hat{B}^2$). Furthermore, using Eq. (3.67), the energy convoluted dimensionless transport coefficient

can be written as

$$\gamma_{33}^{L} = \frac{4}{\sqrt{\pi} l_c v_{te}} \int_{0}^{\infty} dx e^{-x^2} x^2 D_{33}^{L}(x).$$
 (6.23)

According to Eq. (6.11) the collisionality parameter κ^{mono} may be replaced by

$$\kappa^{\text{mono}} = \kappa \frac{3\sqrt{\pi}}{4x^4} Z_{\text{eff}} , \qquad (6.24)$$

where $x = v/v_{te}$, $l_c = v_{te}\tau_{ee}$ and $\kappa = 1/l_c$, respectively. Hence, the dimensionless Lorentz conductivity reads

$$\gamma_{33}^{L} = -\frac{4}{\sqrt{\pi}l_c} \int_{0}^{\infty} dx e^{-x^2} x^2 \frac{x\langle \hat{B}^2 \rangle}{3\kappa} \frac{4x^4}{3\sqrt{\pi}Z_{\text{eff}}}$$

$$= -\frac{16\langle \hat{B}^2 \rangle}{9\pi Z_{\text{eff}}} \int_{0}^{\infty} dx e^{-x^2} x^7. \tag{6.25}$$

If one recalls that

$$\int_{0}^{\infty} \mathrm{d}x x^{n} e^{-x^{2}} = \frac{1}{2} \Gamma\left(\frac{n+1}{2}\right), \quad \text{for} \quad n > -1, \qquad (6.26)$$

the velocity integral appearing in Eq. (6.25) yields $\Gamma(4)/2 = 3$, and the dimensionless Lorentz conductivity within the NEO-2 model is thus found to be

$$\gamma_{33}^{L} = -\frac{16\langle \hat{B}^2 \rangle}{3\pi Z_{\text{eff}}}.$$
 (6.27)

Finally, the dimensional conductivity follows from Eq. (6.6),

$$\sigma_{\text{NEO}}^{L} = -\frac{2n_{e}e^{2}\tau_{ee}}{m_{e}\langle\hat{B}^{2}\rangle}\gamma_{33}^{L}$$

$$= \frac{2n_{e}e^{2}\tau_{ee}}{m_{e}\langle\hat{B}^{2}\rangle}\frac{16\langle\hat{B}^{2}\rangle}{3\pi Z_{\text{eff}}}$$

$$= \frac{32}{3\pi}\frac{n_{e}e^{2}}{m_{e}}\frac{\tau_{ee}}{Z_{\text{eff}}}, \qquad (6.28)$$

which is in agreement with the well-known result for the Spitzer conductivity in the Lorentz limit that can be found in any textbook on plasma physics (see, e.g., References 22 and 57).

6.2 Spitzer function

As a first benchmark for the results derived in Chapter 5 the collision matrix elements are used to calculate the collisional Spitzer function. For these purposes the linearized drift kinetic equation with respect to the first order electron distribution function is to be solved using the full linearized Coulomb collision operator taking into account electron-ion as well as electron-electron collisions. The corresponding solution may then be compared with that by Spitzer and Härm.

In References 45 and 39 the following ansatz for the distribution function was used,

$$f_{sp}(\lambda, x) = f_{e0}(x)\lambda A \frac{D(x)}{A} , \qquad (6.29)$$

with

$$A \equiv -\frac{m_e E v_{te}^2}{2\pi e^3 n_e \ln(qC^2)}. (6.30)$$

The numerical results for the quantity D/A can be found tabulated in [39].

As mentioned above, for purposes of comparison with the Spitzer-Härm results one has to take the limit of a constant magnetic field \hat{B} giving rise to $f_{sp} \neq f(s)$. Thus, within the NEO-2 model the drift kinetic equation has the form [see Eq. (3.26) along with Eq. (3.21) and $A_1 = A_2 = 0$],

$$-\kappa \sum_{m'=0}^{M} \left\{ \nu_{mm'}^{e} \hat{\mathcal{L}} \left[f_{m'}^{\sigma} \right] + \hat{\mathcal{K}}_{mm'}^{e} \left[f_{m'}^{\sigma} \right] + \frac{1}{|\lambda|} D_{mm'}^{e} f_{m'}^{\sigma} \right\} = A_{3} a_{m}^{(3)} q_{3}^{\sigma} , \qquad (6.31)$$

where $A_3 = -(e/T_e)\langle E_{\parallel}\hat{B}\rangle/\langle \hat{B}^2\rangle$, $q_3^{\sigma} = \sigma\hat{B}$, $\kappa = 1/l_c$, $l_c = v_{te}\tau_{ee}$, $v_{te} = \sqrt{2T_e/m_e}$, and $\tau_{ee} = 3m_e^2v_{te}^3/(16\sqrt{\pi}n_ee^4\ln\Lambda)$. The pitch-angle operator and the operator representing the integral part of the Coulomb collision term are given by

$$\hat{\mathcal{L}}\left[f_{m'}^{\sigma}\right] = \frac{1}{2|\lambda|} \frac{\partial}{\partial \lambda} \left(1 - \lambda^{2}\right) \frac{\partial}{\partial \lambda} f_{m'}^{\sigma} \tag{6.32}$$

and

$$\hat{\mathcal{K}}_{mm'}^{e} [f_{m'}^{\sigma}] = \frac{1}{|\lambda|} \sum_{\ell=0}^{L} I_{mm'}^{(\ell)} P_{\ell}(\lambda) \int_{-1}^{1} d\lambda' P_{\ell}(\lambda') f_{m'}^{\sigma}(\lambda'), \tag{6.33}$$

respectively. It is convenient to introduce a normalized distribution function as follows,

$$f_m^{\sigma} = \frac{A_3}{\kappa} \hat{f}_m. \tag{6.34}$$

Bearing in mind Eq. (6.29) one can infer that

$$\hat{f}_m(\lambda) = \lambda c_m = P_1(\lambda)c_m. \tag{6.35}$$

Substituting Eq. (6.35) into Eqs. (6.32) and (6.33) yields

$$|\lambda|\hat{\mathcal{L}}\left[\hat{f}_{m'}\right] = \frac{1}{2}\frac{\partial}{\partial\lambda}\left(1-\lambda^2\right)\frac{\partial}{\partial\lambda}\lambda c_{m'}$$

$$= -\lambda c_{m'} \tag{6.36}$$

and

$$|\lambda|\hat{\mathcal{K}}_{mm'}^{e}\left[\hat{f}_{m'}\right] = \sum_{\ell=0}^{L} I_{mm'}^{(\ell)} P_{\ell}(\lambda) \int_{-1}^{1} d\lambda' P_{\ell}(\lambda') P_{1}(\lambda') c_{m'}$$

$$= \sum_{\ell=0}^{L} I_{mm'}^{(\ell)} P_{\ell}(\lambda) c_{m'} \frac{2}{2\ell+1} \delta_{\ell 1}$$

$$= \frac{2}{3} I_{mm'}^{(1)} c_{m'} \lambda , \qquad (6.37)$$

respectively, where the orthogonality relation for Legendre polynomials [see Eq. (6.17)] has been employed. Using Eqs. (6.35)-(6.37) the drift kinetic equation (6.31) reduces to an algebraic system of equations for the coefficients c_m ,

$$\sum_{m'=0}^{M} \left\{ \nu_{mm'}^{e} - \frac{2}{3} I_{mm'}^{(1)} - D_{mm'}^{e} \right\} c_{m'} = a_{m}^{(3)}, \qquad (6.38)$$

where $\nu_{mm'}^e = \nu_{mm'}^{ee} + Z_{\text{eff}}\nu_{mm'}^{e\infty}$. Upon solving Eq. (6.38) for c_m and recalling that the distribution function is expanded in terms of test functions φ_m ,

$$f_{sp}(x,\lambda) = f_{e0}(x) \sum_{m=0}^{M} f_m^{\sigma}(\lambda) \varphi_m(x), \qquad (6.39)$$

the Spitzer function is determined by the relation

$$f_{sp} = f_{e0}\lambda \frac{A_3}{\kappa} \sum_{m=0}^{M} c_m \varphi_m(x). \tag{6.40}$$

The quantity A_3/κ is related to Eq. (6.30) in the following way,

$$\frac{A_3}{\kappa} = -\frac{e}{T_e} \langle E_{\parallel} \rangle v_{te} \tau_{ee}$$

$$= -\frac{e}{T_e} \langle E_{\parallel} \rangle \frac{3}{4\sqrt{\pi}} \frac{T_e^2}{n_e e^4 \ln \Lambda} \frac{m_e}{m_e} \frac{2}{2}$$

$$= -\frac{\langle E_{\parallel} \rangle v_{te}^2 m_e}{2\pi n_e e^3 \ln \Lambda} \frac{3}{8\sqrt{\pi}} 2\pi$$

$$\equiv A \frac{3\sqrt{\pi}}{4}. \tag{6.41}$$

Therefore, one finally obtains

$$\frac{D}{A} = \frac{3\sqrt{\pi}}{4} \sum_{m=0}^{M} c_m \varphi_m(x) , \qquad (6.42)$$

with the basis functions

$$\varphi_m(x) = \pi^{3/4} \sqrt{\frac{2m!}{\Gamma(m+5/2)}} L_m^{(3/2)}(x^2).$$
(6.43)

The quantity D/A is to be compared with the "exact" numerical result calculated by Spitzer and Härm (see Reference 39). Their result was obtained by integrating numerically the drift kinetic equation (where no expansion of the distribution function was used) which is equivalent to using all the basis functions φ_m , that is M is equal to infinity.

Figure 6.1 shows, in principle, good agreement between the Spitzer-Härm result and the Spitzer function evaluated by means of Eq. (6.42) using four test functions (M=3). However, when zooming in on the x-axis one observes that D/A is negative in the range $0 < x \lesssim 0.21$. This unphysical behavior is still present, although considerably reduced, even when 51 terms have been retained in the expansion of the distribution function (see Figure 6.2). From this one can conclude, that the approximation of the Spitzer function in terms of a few low order associated Laguerre polynomials is only meaningful in the range $x \gtrsim 0.21$.

According to Eq. (3.57) the dimensionless transport coefficient describing the parallel electric conductivity is given by

$$\gamma_{33} = \frac{1}{l_c} \sum_{m=0}^{M} \sum_{\sigma=\pm 1} b_m^{(3)} \left\langle \frac{\hat{B}}{4} \int_0^{1/B} d\eta q_3^{-\sigma} f_m^{\sigma,(3)} \right\rangle$$
 (6.44)

$$= -\frac{1}{l_c} \sum_{m=0}^{M} b_m^{(3)} \left\langle \frac{1}{2} \int_{1}^{1} d\lambda \lambda \hat{B} f_m^{(3)} \right\rangle , \qquad (6.45)$$

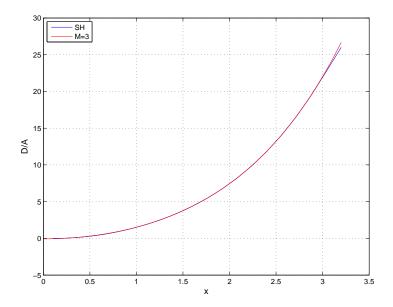


Figure 6.1: Spitzer function, D/A, vs. normalized particle speed, x, for $Z_{\rm eff}=1$. Blue: Spitzer-Härm result, red: result obtained from Eq. (6.42) using M=3.

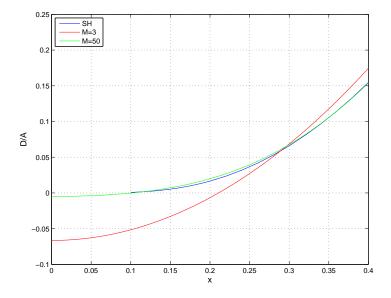


Figure 6.2: A zoomed-in view of Fig. 6.1. In addition: Green curve shows function D/A calculated with 51 test functions.

$Z_{\rm eff}$	γ_E^{SH}	$\gamma_E^{M=1}$	$\gamma_E^{M=2}$	$\gamma_E^{M=10}$
1	0.5816	0.5985	0.5824	0.5820
2	0.6833	0.6999	0.6871	0.6857
4	0.7849	0.7740	0.7847	0.7853
16	0.9225	0.8465	0.9221	0.9234
∞	1	1	1	1

Table 6.1: Spitzer-Härm result vs. Eq. (6.47)

where again Eq. (6.21) has been applied. The quantity $b_m^{(3)}$ can be calculated with the help of Eq. (3.56). Substituting into Eq. (6.45) the assumption $\hat{B} = 1$, and recalling the ansatz $f_m^{(3)} = l_c \lambda c_m$ the transport coefficient γ_{33} can be written as

$$\gamma_{33} = -\sum_{m=0}^{M} b_m^{(3)} \left\langle \frac{1}{2} \int_{-1}^{1} d\lambda \lambda^2 c_m \right\rangle$$

$$= -\sum_{m=0}^{M} b_m^{(3)} c_m \frac{1}{2} \int_{-1}^{1} d\lambda \lambda^2$$

$$= -\frac{1}{3} \sum_{m=0}^{M} b_m^{(3)} c_m. \qquad (6.46)$$

In virtue of Eq. (6.8) the Spitzer-Härm coefficient γ_E including electronelectron effects can thus be computed by means of

$$\gamma_{E} = -\frac{3\pi Z_{\text{eff}}}{16} \gamma_{33}$$

$$= \frac{\pi}{16} Z_{\text{eff}} \sum_{m=0}^{M} b_{m}^{(3)} c_{m}.$$
(6.47)

Table 6.1 presents the "exact" Spitzer-Härm result for the normalized conductivity γ_E for several values of $Z_{\rm eff}$ as well as the corresponding semi-analytical result calculated from Eq. (6.47) depending on the number M of terms included in the polynomial expansion of the distribution function [see Eq. (6.39)]. One can see that sufficient accuracy is already obtained by taking M=2 [the results of Eq. (6.47) for M=1 match the Spitzer-Härm results to within 3-8% and for M=2 to within 0.03-0.56%].

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These results confirm the correctness of the collision matrix elements for the full linearized Coulomb operator numerically evaluated from Eqs. (5.188), (5.220), (5.230) and (5.346), respectively.

Chapter 7

Comparison to results reported in literature

In this chapter the neoclassical transport coefficients for an axisymmetric toroidal system are computed in the limit of low collisionality using analytical results which are most widely used in the plasma physics literature. These results are compared to the corresponding numerical results evaluated by means of the NEO-2 code. The expressions representing the neoclassical transport matrix within the NEO-2 model have already been derived in Chapter 3 and are included here again for completeness.

The electron transport coefficients L_{jk}^e have been defined through

$$I_j = -\sum_{k=1}^3 L_{jk}^e A_k, (7.1)$$

relating the fluxes

$$I_1 \equiv \Gamma_e , \qquad I_2 \equiv \frac{Q_e}{T_e} , \qquad I_3 \equiv -\frac{\langle j_{\parallel} \hat{B} \rangle}{e} ,$$
 (7.2)

to the thermodynamical forces

$$A_1(r) = \left(\frac{1}{n_e} \frac{\mathrm{d}n_e}{\mathrm{d}\psi} - \frac{3}{2T_e} \frac{\mathrm{d}T_e}{\mathrm{d}\psi} - \frac{e}{T_e} \frac{\mathrm{d}\Phi}{\mathrm{d}\psi}\right) \langle |\nabla \psi| \rangle \tag{7.3}$$

$$A_2(r) = \frac{1}{T_e} \frac{\mathrm{d}T_e}{\mathrm{d}\psi} \langle |\nabla \psi| \rangle \tag{7.4}$$

$$A_3(r) = -\frac{e}{T_e} \frac{\langle E_{\parallel}^{(A)} \hat{B} \rangle}{\langle \hat{B}^2 \rangle}, \tag{7.5}$$

where $\hat{B} = B/B_0$ and B_0 denotes some reference magnetic field. The dimensionless transport matrix, γ_{ik} , has been defined in the form

$$L_{jk}^{e} = \frac{n_e}{\tau_{ee}} \hat{\beta}_j \hat{\beta}_k \gamma_{jk}, \tag{7.6}$$

where

$$\hat{\beta}_1 = \hat{\beta}_2 = \rho, \qquad \hat{\beta}_3 = l_c, \tag{7.7}$$

$$\hat{\beta}_1 = \hat{\beta}_2 = \rho, \quad \hat{\beta}_3 = l_c,$$

$$\rho = \frac{v_{te}}{\omega_{c0}}, \quad \omega_{c0} = \frac{eB_0}{m_e c}, \quad l_c = v_{te} \tau_{ee},$$
(7.7)

and

$$\tau_{ee} = \frac{3m_e^2 v_{te}^3}{16\sqrt{\pi}n_e e^4 \ln \Lambda}$$
 (7.9)

is the collision time, respectively (for details see Chapters 3.1 and 3.2).

In the following the neoclassical electron transport matrix γ_{ik} for the standard tokamak test configuration (see Appendix F) evaluated using the NEO-2 code is benchmarked with the corresponding analytical results obtained by Balescu [37,56], and Hirshman [59] in the low-collisionality (banana) regime (cf. Chapter 7.5) as well as with the results reported by Hinton and Hazeltine [60] and Sauter, Angioni and Lin-Liu [38, 61–63] which are valid for arbitrary collisionality regime (see also Chapter 8.2).

Balescu 7.1

The results for the neoclassical transport matrix in the low collisionality limit were derived in the so-called twenty-one moment (21M) approximation (applying an approximate collision operator). This corresponds to the fact that the expansion of the distribution function in Laguerre polynomials is truncated at the level M=2 (that is to say, three polynomials are retained). For details see References 37 and 56. Furthermore, the results are valid for arbitrary aspect ratio.

In [37] the dimensional electron banana transport equations representing the averaged radial particle flux, $\langle \Gamma_r^e \rangle_b$, the averaged radial heat flux, $\langle q_r^e \rangle_b$ and the averaged parallel electric current density, $\langle j_{\parallel}B\rangle_{b}$, have been written as follows,

$$\left\langle \Gamma_{r}^{e} \right\rangle_{b} = L_{11}^{ee} X_{1}^{e} + L_{13}^{ee} X_{3}^{e} + L_{13}^{ei} X_{3}^{i} + L_{1E}^{e} X_{E}$$
 (7.10)

$$\frac{1}{T_e} \langle q_r^e \rangle_b = L_{31}^{ee} X_1^e + L_{33}^{ee} X_3^e + L_{33}^{ei} X_3^i + L_{3E}^e X_E$$
 (7.11)

$$\frac{1}{\mathscr{B}_0^{\text{Bal}}} \langle j_{\parallel} B \rangle_b = L_{E1}^e X_1^e + L_{E3}^e X_3^e + L_{E3}^i X_3^i + L_{EE} X_E, \tag{7.12}$$

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with the thermodynamic forces defined by

$$X_1^e \equiv X_1 = -\frac{1}{n_e T_e} \nabla_r P \tag{7.13}$$

$$X_3^e \equiv X_2 = -\frac{1}{T_e} \nabla_r T_e \tag{7.14}$$

$$X_3^i \equiv X_3 = -\frac{1}{T_i} \nabla_r T_i \tag{7.15}$$

$$X_E \equiv X_4 = \frac{1}{\mathscr{B}_0^{\text{Bal}}} \langle E_{\parallel}^{(A)} B \rangle.$$
 (7.16)

To leading order in the tokamak standard model used by Balescu one can replace ∇_r by $\partial/\partial r$ [37]. In the present work the electron part of the neoclassical transport matrix, γ_{jk} , has been determined assuming immobile background ions. Thus, $T_i \equiv 0$ and the coefficients L_{13}^{ei} , L_{33}^{ei} and L_{E3}^{i} do not contribute. The dimensional electron transport coefficients are given by (see Table 3.4 in Reference 37)

$$L_{11}^{ee} = \frac{n_e \rho_{e0}^2}{\tau_e} \mathcal{J}^2 \frac{1}{2} \varphi l_{11}^{ee}(\varphi)$$
 (7.17)

$$L_{33}^{ee} = \frac{n_e \rho_{e0}^2}{\tau_e} \mathcal{J}^2 \frac{5}{4} \varphi l_{33}^{ee}(\varphi)$$
 (7.18)

$$L_{13}^{ee} = L_{31}^{ee} = \frac{n_e \rho_{e0}^2}{\tau_e} \mathcal{J}^2 \frac{\sqrt{5}}{2\sqrt{2}} \varphi l_{13}^{ee}(\varphi)$$
 (7.19)

and

$$L_{1E}^e = -L_{E1}^e = -\frac{n_e T_e c}{\mathscr{B}_0^{\text{Bal}}} \mathscr{J} \varphi l_{1E}^e(\varphi)$$
 (7.20)

$$L_{3E}^e = -L_{E3}^e = -\frac{n_e T_e c}{\mathscr{B}_0^{\text{Bal}}} \mathscr{J} \sqrt{\frac{5}{2}} \varphi l_{3E}^e(\varphi)$$
 (7.21)

$$L_{EE} = \frac{n_e e^2}{m_e} \tau_e \varphi l_{EE}(\varphi), \qquad (7.22)$$

where Eqs. (7.17)-(7.19) are the pure diffusive coefficients and Eqs. (7.20)-(7.22) represent the electrical coefficients. Here, τ_e is the electron relaxation time

$$\tau_e = \frac{3}{16\sqrt{\pi}} \frac{v_{te}^3 m_e^2}{n_i Z^2 e^4 \ln \Lambda},\tag{7.23}$$

the neoclassical factor $\varphi = f_t/f_c$, where f_t is the trapped particle fraction and $f_c = 1 - f_t$, the surface averaged reference magnetic field $\mathscr{B}_0^{\text{Bal}} = \langle B^2 \rangle^{1/2}$,

the reference Larmor radius $\rho_{e0}^2 = v_{te}^2/\Omega_{e0}^2$ where $v_{te}^2 = 2T_e/m_e$ and $\Omega_{e0}^2 = (e\mathscr{B}_0^{\rm Bal}/m_ec)^2$, the scale factor $l_r = \sqrt{g_{rr}} = 1$, the effective poloidal field is $\mathscr{B}_P = (1/R_0) \mathrm{d}\chi(r)/\mathrm{d}r$ and $\mathscr{J} = \mathscr{J}l_r/(R_0\mathscr{B}_P)$. The quantity \mathscr{J} can also be calculated using the contravariant angular magnetic field components, respectively, that is $\mathscr{J} = \hat{B}^{\varphi}/\hat{B}^{\theta}$ and χ is the poloidal flux.

In the case of the standard tokamak (see Appendix F), where the magnetic field is expressed as

$$\mathbf{B}(r,\theta) = \frac{\mathscr{B}_0}{1 + \epsilon(r)\cos\theta} \left[\iota(r)\epsilon(r)\,\hat{\mathbf{e}}_\theta + \sqrt{1 - \epsilon(r)^2}\,\hat{\mathbf{e}}_\varphi \right],\tag{7.24}$$

one gets for these geometrical factors $d\psi/dr = \mathcal{B}_0 r$ where ψ is the toroidal flux, $\chi'/\psi' = \iota$ denotes the rotational transform, $\mathcal{B}_P = (\iota/R_0)\mathcal{B}_0 r = \iota \epsilon \mathcal{B}_0$, $\epsilon = r/R_0$ is the inverse aspect ratio,

$$\mathscr{J} \equiv \frac{\hat{B}^{\varphi}}{\hat{B}^{\theta}} = \frac{\sqrt{1 - \epsilon^2}}{\iota \epsilon},\tag{7.25}$$

and the trapped particle fraction is evaluated by means of a very accurate approximation proposed in Reference 64 yielding

$$f_t \cong 1.4624\sqrt{\epsilon} - 0.2424\epsilon^{3/2} + \mathcal{O}(\epsilon^2).$$
 (7.26)

The reference magnetic field is chosen to be the m=0 Fourier mode of magnetic field module B in Boozer coordinates (see Appendix F.3.2)

$$B(\theta_B) = \sum_m b_m \cos \theta_B. \tag{7.27}$$

Recalling Eqs. (7.6)-(7.8) the transport coefficient in Eq. (7.17) can be expressed as

$$L_{11}^{ee} = \frac{n_e \rho^2}{\tau_{ee}} \underbrace{\frac{\tau_{ee}}{\tau_e} \frac{\rho_{e0}^2}{\rho^2} \mathscr{J}^2 \frac{1}{2} \varphi l_{11}^{ee}(\varphi)}_{\gamma_{11}^{\text{Bal}}}.$$
 (7.28)

Upon replacing the ratio of electron collision times τ_{ee}/τ_e by $Z_{\rm eff}$ as well as the ratio of Larmor radii by

$$\frac{\rho_{e0}^2}{\rho^2} = \frac{b_0^2}{\langle B^2 \rangle} = \frac{1}{\langle \hat{B}^2 \rangle} = \frac{1}{(1 - \epsilon^2)^{3/2}}, \tag{7.29}$$

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the dimensionless banana transport coefficient $\gamma_{11}^{'\text{Bal}}$ becomes

$$\gamma_{11}^{'\text{Bal}} = \frac{Z_{\text{eff}}}{\langle \hat{B}^2 \rangle} \mathscr{J}^2 \frac{\varphi}{2} l_{11}^{ee}(\varphi)$$
 (7.30)

$$= \frac{Z_{\text{eff}}}{2t^2\epsilon^2\sqrt{1-\epsilon^2}} \frac{f_t}{f_c} l_{11}^{ee}(f_t/f_c)$$
 (7.31)

where in the last equation the geometrical factors for the standard tokamak have been substituted. Similarly, Eqs. (7.18) and (7.19) lead to

$$\gamma_{12}^{'\text{Bal}} = \gamma_{21}^{'\text{Bal}} = \frac{Z_{\text{eff}}}{\langle \hat{B}^2 \rangle} \mathcal{J}^2 \sqrt{\frac{5}{2}} \frac{\varphi}{2} l_{13}^{ee}(\varphi)$$
 (7.32)

$$= \sqrt{\frac{5}{8}} \frac{Z_{\text{eff}}}{t^2 \epsilon^2 \sqrt{1 - \epsilon^2}} \frac{f_t}{f_c} l_{13}^{ee}(f_t/f_c), \tag{7.33}$$

and

$$\gamma_{22}^{'\text{Bal}} = \frac{Z_{\text{eff}}}{\langle \hat{B}^2 \rangle} \mathscr{J}^2 \frac{5}{2} \frac{\varphi}{2} l_{33}^{ee}(\varphi)$$
 (7.34)

$$= \frac{5}{4} \frac{Z_{\text{eff}}}{t^2 \epsilon^2 \sqrt{1 - \epsilon^2}} \frac{f_t}{f_c} l_{33}^{ee}(f_t/f_c), \tag{7.35}$$

respectively. Using $X_E = -B_0 T_e \langle \hat{B}^2 \rangle A_3 / (\mathcal{B}_0^{\text{Bal}} e) = -\mathcal{B}_0^{\text{Bal}} T_e A_3 / (B_0 e)$ the last term on the RHS of Eq. (7.10) yields

$$L_{1E}^{e}X_{E} = -L_{1E}^{e} \frac{\mathscr{B}_{0}^{\text{Bal}}}{B_{0}} \frac{T_{e}}{e} A_{3}(r), \tag{7.36}$$

from which it follows that the dimensionless transport coefficient characterizing the Ware-Galeev pinch effect can be written as

$$\gamma_{13}^{'\text{Bal}} = -\frac{\tau_{ee}}{n_e \rho l_c} \frac{n_e c}{\mathcal{B}_0^{\text{Bal}}} \mathscr{J} \varphi l_{1E}^e(\varphi) \frac{\mathcal{B}_0^{\text{Bal}} T_e}{B_0 e}
= -\frac{\varphi}{2} \mathscr{J} l_{1E}^e(\varphi)$$

$$= -\frac{\sqrt{1 - \epsilon^2}}{2t\epsilon} \frac{f_t}{f_c} l_{1E}^e(f_t/f_c).$$
(7.38)

Likewise, from Eq. (7.11) one gets

$$\gamma_{23}^{'\text{Bal}} = -\sqrt{\frac{5}{2}} \mathscr{J} \frac{\varphi}{2} l_{3E}^e(\varphi) \tag{7.39}$$

$$= -\sqrt{\frac{5}{8}} \frac{\sqrt{1-\epsilon^2}}{\epsilon} \frac{f_t}{f_c} l_{3E}^e(f_t/f_c). \tag{7.40}$$

The transport coefficient representing the bootstrap current may be derived, upon recalling the definition of $I_3 \equiv -\langle j_{\parallel} \hat{B} \rangle / e$, by means of the first term on the RHS of Eq.(7.12),

$$-\frac{\mathscr{B}_{0}^{\text{Bal}}}{B_{0}e}L_{E1}^{e}X_{1}^{e} = \frac{\mathscr{B}_{0}^{\text{Bal}}}{B_{0}e}L_{E1}^{e}\frac{1}{n_{e}T_{e}}\left(\frac{\partial P}{\partial r}\right),\tag{7.41}$$

leading to

$$\gamma_{31}^{'\text{Bal}} = -\frac{\tau_{ee}}{n_e \rho l_c} \frac{\mathscr{B}_0^{\text{Bal}}}{B_0 e} \frac{n_e T_e c}{\mathscr{B}_0^{\text{Bal}}} \mathscr{J} \varphi l_{1E}^e(\varphi)
= -\frac{\varphi}{2} \mathscr{J} l_{1E}^e(\varphi)
= -\frac{\sqrt{1 - \epsilon^2}}{2t\epsilon} \frac{f_t}{f_c} l_{1E}^e(f_t/f_c).$$
(7.42)

Similarly, the coefficient $\gamma_{32}^{'\text{Bal}}$ can be expressed as

$$\gamma_{32}^{'\text{Bal}} = -\sqrt{\frac{5}{2}} \mathscr{J} \frac{\varphi}{2} l_{3E}^{e}(\varphi)$$

$$= -\sqrt{\frac{5}{8}} \frac{\sqrt{1 - \epsilon^{2}}}{t\epsilon} \frac{f_{t}}{f_{c}} l_{3E}^{e}(f_{t}/f_{c}),$$

$$(7.44)$$

and the electrical conductivity coefficient is obtained from the last term on the RHS of Eq. (7.12),

$$-\frac{\mathscr{B}_0^{\text{Bal}}}{B_0 e} L_{EE} X_E = L_{EE} \frac{T_e \langle \hat{B}^2 \rangle}{e^2} A_3 \tag{7.46}$$

yielding

$$\gamma_{33}^{'\text{Bal}} = -\frac{\tau_{ee}}{n_e l_c^2} \frac{n_e e^2}{m_e} \tau_e \varphi l_{EE}(\varphi) \frac{T_e \langle \hat{B}^2 \rangle}{e^2}
= -\frac{\tau_e}{\tau_{ee}} \frac{\langle \hat{B}^2 \rangle}{2} \varphi l_{EE}(\varphi)
= -\frac{\langle \hat{B}^2 \rangle}{2Z_{\text{eff}}} \varphi l_{EE}(\varphi).$$
(7.47)

To compare with NEO-2 results one has to add the classical electrical conductivity σ (which is given in Table 3.2 of Reference 56),

$$\gamma_{33}^{'\text{Bal}} = -\frac{\langle \hat{B}^2 \rangle}{2Z_{\text{eff}}} \left[\sigma(Z_{\text{eff}}) + \varphi l_{EE}(\varphi) \right]. \tag{7.49}$$

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In contrast to Chapter 3.2 where the second flux has been defined as the surface averaged total radial flux of energy, $I_2 \equiv Q_e/T_e$, Balescu defined I_2 via the flux surface averaged radial heat flux q_e , that is $I_2 \equiv q_e/T_e$. Therefore, the transport matrix $\gamma_{jk}^{'\text{Bal}}$ has to be transformed using the following equations (see also Chapter 3.3)

$$\gamma_{11}^{\text{Bal}} = \gamma_{11}^{'\text{Bal}}$$
(7.50)

$$\gamma_{11}^{\text{Bal}} = \gamma_{11}^{'\text{Bal}}$$
(7.50)
$$\gamma_{12}^{\text{Bal}} = \gamma_{12}^{'\text{Bal}} + \frac{5}{2}\gamma_{11}^{'\text{Bal}}$$
(7.51)

$$\gamma_{22}^{\text{Bal}} = \gamma_{22}^{'\text{Bal}} + 5\gamma_{12}^{'\text{Bal}} + \frac{25}{4}\gamma_{11}^{'\text{Bal}}$$
(7.52)

$$\gamma_{13}^{\text{Bal}} = \gamma_{13}^{'\text{Bal}} \tag{7.53}$$

$$\gamma_{23}^{\text{Bal}} = \gamma_{23}^{'\text{Bal}} + \frac{5}{2}\gamma_{13}^{'\text{Bal}}$$
(7.54)

$$\gamma_{33}^{\text{Bal}} = \gamma_{33}^{'\text{Bal}}.$$
(7.55)

These coefficients are to be compared to the results of the NEO-2 code.

7.2 Hirshman

In Reference 59, Hirshman computed the bootstrap current in tokamaks, valid for arbitrary values of aspect ratio (and flux surface geometry) and effective ion charge in the collisionless limit (see also [22]) using an approximate collision operator [30]. The results are equivalent to the thirteen moment (13M) approximation [37] (retaining only two Laguerre polynomials in the expansion of the distribution function).

The expression for the parallel current density has been given as [22]

$$\langle j_{\parallel}B\rangle = -\frac{Ip_e}{D} \left[d_1 \frac{1}{p_e} \frac{\mathrm{d}p_e}{\mathrm{d}\chi} + d_2 \frac{1}{T_e} \frac{\mathrm{d}T_e}{\mathrm{d}\chi} + d_1 \frac{T_i}{ZT_e} \left(\frac{1}{p_i} \frac{\mathrm{d}p_i}{\mathrm{d}\chi} + \alpha_i \frac{1}{T_i} \frac{\mathrm{d}T_i}{\mathrm{d}\chi} \right) \right] + \frac{d_3}{D} \frac{n_e e^2 \tau_{ee}}{m_e} \langle E_{\parallel}B \rangle , \qquad (7.56)$$

where χ is the poloidal flux and the quantities d_1 , d_2 and D are as follows

$$d_1(x, Z) = x \left[0.754 + 2.21Z + Z^2 + x \left(0.348 + 1.243Z + Z^2 \right) \right] (7.57)$$

$$d_2(x,Z) = -x(0.884 + 2.074Z) (7.58)$$

$$d_3(x,Z) = 1.414 + 3.25Z + x(1.387 + 3.25Z)$$
 (7.59)

$$D(x,Z) = 1.414Z + Z^{2} + x (0.754 + 2.657Z + 2Z^{2}) +x^{2} (0.348 + 1.243Z + Z^{2}),$$
 (7.60)

with Z being the effective ion charge and $x = f_t/f_c$ represents the ratio between the trapped and circulating particles and $\alpha_i = -1.173/(1 + 0.462x)$ is the poloidal rotation coefficient [22]. Using $t = \chi'/\psi' = d\chi/d\psi$, $d/d\chi = (1/t)d/d\psi$, $\hat{B} = B/b_0$ and $-\langle j_{\parallel}\hat{B}\rangle/e \equiv I_3$, respectively, Eq. (7.56) can be recast to the form

$$I_{3}(\psi) = \frac{Ip_{e}}{eb_{0}D_{t}} \left[d_{1}\frac{1}{p_{e}}\frac{\mathrm{d}p_{e}}{\mathrm{d}\psi} + d_{2}\frac{1}{T_{e}}\frac{\mathrm{d}T_{e}}{\mathrm{d}\psi} + d_{1}\frac{T_{i}}{ZT_{e}} \left(\frac{1}{p_{i}}\frac{\mathrm{d}p_{i}}{\mathrm{d}\psi} + \alpha_{i}\frac{1}{T_{i}}\frac{\mathrm{d}T_{i}}{\mathrm{d}\psi} \right) \right] - \frac{d_{3}}{D}\frac{n_{e}e\tau_{ee}T_{e}}{m_{e}T_{e}} \langle E_{\parallel}\hat{B}\rangle .$$

$$(7.61)$$

Upon applying

$$\frac{p_i}{p_e} = \frac{n_i T_i}{n_e T_e} = \frac{T_i}{Z T_e},$$
 (7.62)

where the quasi-neutrality condition $n_e = Zn_i$ has been used and

$$\frac{\mathrm{d}\ln p_e}{\mathrm{d}\psi} + \frac{T_i}{ZT_e} \frac{\mathrm{d}\ln p_i}{\mathrm{d}\psi} = \frac{p}{p_e} \frac{\mathrm{d}\ln p}{\mathrm{d}\psi},\tag{7.63}$$

one obtains

$$I_{3}(r) = \frac{Ip_{e}}{eb_{0}D_{t}\langle|\nabla\psi|\rangle} \left(d_{1}A_{1}^{'e} + d_{2}A_{2}^{'e} + d_{1}\frac{T_{i}}{ZT_{e}}\alpha_{i}A_{2}^{'i}\right) + \frac{d_{3}}{D} \frac{n_{e}\tau_{ee}T_{e}}{m_{e}}\langle\hat{B}^{2}\rangle A_{3}^{'e},$$
(7.64)

with the driving forces

$$A_1^{'e}(r) = \frac{1}{p_e} \frac{\mathrm{d}p}{\mathrm{d}\psi} \langle |\nabla\psi| \rangle \tag{7.65}$$

$$A_2^{'e}(r) = \frac{1}{T_e} \frac{\mathrm{d}T_e}{\mathrm{d}\psi} \langle |\nabla\psi| \rangle \tag{7.66}$$

$$A_2^{'i}(r) = \frac{1}{T_i} \frac{\mathrm{d}T_i}{\mathrm{d}\psi} \langle |\nabla \psi| \rangle \tag{7.67}$$

$$A_3^{'e}(r) = -\frac{e}{T_e} \frac{\langle E_{\parallel} \hat{B} \rangle}{\langle \hat{B}^2 \rangle}. \tag{7.68}$$

In order to compare with the NEO-2 model the ion temperature is assumed to be zero, that is $T_i = 0$. In accordance with Eq. (7.1) it follows that

$$L_{3k}^{'ee} = -\frac{Ip_e}{eb_0t\langle|\nabla\psi|\rangle}\frac{d_k}{D}$$

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$$= -\frac{In_e T_e}{eb_0 t \langle |\nabla \psi| \rangle} \frac{d_k}{D} \frac{2m_e}{2m_e}$$

$$= \frac{n_e v_{te}^2}{\omega_{c0}} \underbrace{\left(-\frac{I}{2t \langle |\nabla \psi| \rangle} \frac{d_k}{D}\right)}_{\gamma_{3k}^{ee}}, \quad \text{for } k = 1, 2, \quad (7.69)$$

and the transport coefficient representing the electrical conductivity is expressed as

$$L_{33}^{'ee} = -\frac{n_e \tau_{ee} T_e}{m_e} \langle \hat{B}^2 \rangle \frac{d_3}{D}$$

$$= n_e v_{te}^2 \tau_{ee} \underbrace{\left(-\frac{\langle \hat{B}^2 \rangle}{2} \frac{d_3}{D}\right)}_{\gamma_{ee}^{'ee}}.$$
(7.70)

Therefore, the dimensionless transport coefficients become

$$\gamma_{3k}^{'ee} = -\frac{J}{2\iota\langle|\nabla\psi|\rangle}\frac{d_k}{D} \tag{7.71}$$

$$= -\frac{\sqrt{1 - \epsilon^2}}{2\epsilon t} \frac{d_k}{D}, \quad \text{for} \quad k = 1, 2,$$
 (7.72)

where, for the standard tokamak case, I has been replaced by $J = \mathcal{B}_0 R_0$ $\sqrt{1-\epsilon^2}$ as well as $\langle |\nabla \psi| \rangle = \epsilon \mathscr{B}_0 R_0$ (see Appendix F) and

$$\gamma_{33}^{'ee} = -\frac{\langle \hat{B}^2 \rangle}{2} \frac{d_3}{D} \tag{7.73}$$

$$= -\frac{(1-\epsilon^2)^{3/2}}{2}\frac{d_3}{D},\tag{7.74}$$

respectively, where Eq. (7.29) has been substituted. Finally, the electron transport coefficients with respect to the radial density and temperature gradients and the parallel electric field are

$$\gamma_{31}^{ee} = \gamma_{31}^{'ee} \tag{7.75}$$

$$\gamma_{31}^{ee} = \gamma_{31}^{'ee}$$

$$\gamma_{32}^{ee} = \gamma_{32}^{'ee} + \frac{5}{2}\gamma_{31}^{'ee}$$
(7.75)

$$\gamma_{33}^{ee} = \gamma_{33}^{'ee}.$$
(7.77)

In Reference 65 Hirshman, Sigmar and Clarke calculated the neoclassical transport matrix of a multispecies plasma in the low collision frequency regime for arbitrary aspect ratios where the averaged total cross-field fluxes of particles and energy in terms of the thermodynamic forces have been presented in the form

$$\Gamma_a(\chi) = \sum_{b:n=1,2} L_{1n}^{ab} A_{nb}(\chi)$$
 (7.78)

$$\frac{Q_a}{T_a}(\chi) = \sum_{b:n=1,2} L_{2n}^{ab} A_{nb}(\chi), \tag{7.79}$$

with $A_{1a} = \partial \ln n_a/\partial \chi - (3/2)\partial \ln T_a/\partial \chi$ and $A_{2a} = \partial \ln T_a/\partial \chi$, respectively. Here, a plasma composed of electrons and a single ion species, with charge Z_i , is considered.

The diffusive transport coefficients have been obtained using the ansatz

$$L_{mn}^{ab} = (F_t)^2 L_{mn}^{ab}(f_c \to 0) + F_c L_{mn}^{ab}(f_t \to 0), \quad \text{for} \quad m, n = 1, 2, \quad (7.80)$$

where $F_c = f_c/(\langle B^2 \rangle \langle B^{-2} \rangle)$, $F_t = 1 - F_c$ and the coefficients for the small aspect ratio limit, that is $f_c \to 0$, read

$$L_{11}^{aa} = -\frac{\sum_{k \neq a} \{\nu_s^{ak}\}}{\{\nu_s^a\}} L_a^* \tag{7.81}$$

$$L_{12}^{aa} = L_{21}^{aa} = -\frac{\sum_{k \neq a} \{x^2 \nu_s^{ak}\}}{\{\nu_s^a\}} L_a^*$$
(7.82)

$$L_{22}^{aa} = \left[\frac{\{x^2 \nu_s^{aa}\}^2}{\{\nu_s^{aa}\} \{\nu_s^a\}} - \frac{\{x^4 \nu_s^a\}}{\{\nu_s^a\}} + \frac{\{x^4 \nu_h^{aa}\} + \{x^4 \nu_k^a\}}{\{\nu_s^a\}} \right] L_a^*. \quad (7.83)$$

The velocity space averages (indicated by curly brackets) of the slowing down frequency, $\nu_s^a = \sum_b \nu_s^{ab}$, are given in Eqs. (45a)-(45e) of Reference 65 and the quantity $L_a^* \equiv n_a J^2 v_{ta}^2 B_0^2 \langle B^{-2} \rangle \{ \nu_s^a \} / (2\omega_{c0}^2)$. The coefficients for the large aspect ratio case, $f_t \to 0$, are defined as follows

$$L_{11}^{aa} = -\frac{\sum_{k \neq a} m_k n_k \{\nu_D^k\}}{\sum_k m_k n_k \{\nu_D^k\}} L_a$$
 (7.84)

$$L_{12}^{aa} = L_{21}^{aa} = \frac{\{x^2 \nu_D^a\}}{\{\nu_D^a\}} L_{11}^{aa}$$
(7.85)

$$L_{22}^{aa} = \frac{\{x^2 \nu_D^a\}}{\{\nu_D^a\}} L_{12}^{aa} - \frac{\{x^2 \nu_D^a\}}{\{\nu_D^a\}} L_a \left(\frac{\{x^4 \nu_D^a\}}{\{x^2 \nu_D^a\}} - \frac{\{x^2 \nu_D^a\}}{\{\nu_D^a\}}\right), \quad (7.86)$$

with the velocity space averages of the deflection frequency, $\nu_D^a = \sum_b \nu_D^{ab}$, presented in Eqs. (33a)-(33c) of [65] and $L_a \equiv f_t n_a J^2 v_{ta}^2 B_0^2 \{\nu_D^a\}/(2\omega_{c0}^2 \langle B^2 \rangle)$.

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Upon comparing Eqs. (7.78)-(7.86) with the corresponding quantities used within the NEO-2 model [see Eqs. (7.1)-(7.8)] one arrives at the following expressions for the modified dimensionless diffusive transport coefficients

$$\gamma_{mn}^{ee,\text{mod}} = (F_t)^2 \gamma_{mn}^{ee,c} + F_c \gamma_{mn}^{ee,t}, \tag{7.87}$$

where $\gamma_{mn}^{ee,c} \equiv -\tau_{ee} L_{mn}^{ee}(f_c \to 0)/(n_e \rho^2 t^2 \langle |\nabla \psi| \rangle^2)$ and, accordingly, $\gamma_{mn}^{ee,t} \equiv -\tau_{ee} L_{mn}^{ee}(f_t \to 0)/(n_e \rho^2 t^2 \langle |\nabla \psi| \rangle^2)$, with

$$\gamma_{11}^{ee,c} = \frac{J^2 \langle \hat{B}^{-2} \rangle}{2t^2 \langle |\nabla \psi| \rangle^2} \frac{\tau_{ee}}{\tau_{ei}} \{ \nu_s^{ei} \tau_{ei} \}$$
 (7.88)

$$\gamma_{12}^{ee,c} = \gamma_{21}^{ee,c} = \frac{J^2 \langle \hat{B}^{-2} \rangle}{2t^2 \langle |\nabla \psi| \rangle^2} \frac{\tau_{ee}}{\tau_{ei}} \{ x^2 \nu_s^{ei} \tau_{ei} \}$$
 (7.89)

$$\gamma_{22}^{ee,c} = -\frac{J^2 \langle \hat{B}^{-2} \rangle}{2t^2 \langle |\nabla \psi| \rangle^2} \left[\frac{\{x^2 \nu_s^{ee} \tau_{ee}\}^2}{\{\nu_s^{ee} \tau_{ee}\}} - \{x^4 \nu_s^{ee} \tau_{ee}\} - \frac{\tau_{ee}}{\tau_{ei}} \{x^4 \nu_s^{ei} \tau_{ei}\} \right] + \{x^4 \nu_h^{ee} \tau_{ee}\} + \{x^4 \nu_k^{ee} \tau_{ee}\} + \frac{\tau_{ee}}{\tau_{ei}} \{x^4 \nu_k^{ei} \tau_{ei}\} , \qquad (7.90)$$

and

$$\gamma_{11}^{ee,t} = \frac{f_t J^2}{2\langle \hat{B}^2 \rangle_t^2 \langle |\nabla \psi| \rangle^2} \frac{\{\nu_D^{ee} \tau_{ee}\} + \frac{\tau_{ee}}{\tau_{ei}} \{\nu_D^{ei} \tau_{ei}\}}{1 + R_D^{ei}}$$
(7.91)

$$\gamma_{12}^{ee,t} = \gamma_{21}^{ee,t} = \frac{f_t J^2}{2\langle \hat{B}^2 \rangle_t^2 \langle |\nabla \psi| \rangle^2} \frac{\{x^2 \nu_D^{ee} \tau_{ee}\} + \frac{\tau_{ee}}{\tau_{ei}} \{x^2 \nu_D^{ei} \tau_{ei}\}}{1 + R_D^{ei}}$$
(7.92)

$$\gamma_{22}^{ee,t} = \frac{f_t J^2}{2\langle \hat{B}^2 \rangle t^2 \langle |\nabla \psi| \rangle^2} \left[\{ x^4 \nu_D^{ee} \tau_{ee} \} + \frac{\tau_{ee}}{\tau_{ei}} \{ x^4 \nu_D^{ei} \tau_{ei} \} \right]$$

$$-\frac{\left(\left\{x^{2}\nu_{D}^{ee}\tau_{ee}\right\} + \frac{\tau_{ee}}{\tau_{ei}}\left\{x^{2}\nu_{D}^{ei}\tau_{ei}\right\}\right)^{2}}{\left\{\nu_{D}^{ee}\tau_{ee}\right\} + \frac{\tau_{ee}}{\tau_{ei}}\left\{\nu_{D}^{ei}\tau_{ei}\right\}} \frac{R_{D}^{ei}}{(1 + R_{D}^{ei})}\right],\tag{7.93}$$

respectively, and where the abbreviation

$$R_{D}^{ei} \equiv \frac{m_{e}n_{e}}{m_{i}n_{i}} \frac{\{\nu_{D}^{e}\}}{\{\nu_{D}^{i}\}}$$

$$= \frac{1}{Z_{i}} \sqrt{\frac{m_{e}}{m_{i}}} \left[\frac{\{\nu_{D}^{ee}\tau_{ee}\} + \frac{\tau_{ee}}{\tau_{ei}} \{\nu_{D}^{ei}\tau_{ei}\}}{\{\nu_{D}^{ie}\tau_{ie}\} + \frac{\tau_{ie}}{\tau_{ie}} \{\nu_{D}^{ii}\tau_{ii}\}} \right]$$
(7.94)

has been used. Assuming quasi-neutrality, that is $n_e = Z_i n_i$, the ratios of the collision times, τ_{ee}/τ_{ei} as well as τ_{ie}/τ_{ii} , can be substituted by Z_i . In the case of the standard tokamak $J^2/\langle |\nabla \psi| \rangle^2 = (1 - \epsilon^2)/\epsilon^2$, $B_0 \equiv b_0$, $\langle \hat{B}^{-2} \rangle = (2 + 3\epsilon^2)/[2(1 - \epsilon^2)^2]$, $\langle \hat{B}^2 \rangle = (1 - \epsilon^2)^{3/2}$ and the trapped particle fraction f_t has been given in Eq. (7.26).

7.3 Hinton-Hazeltine

The next neoclassical transport model to be addressed is the one obtained by Hinton and Hazeltine. In Reference 60 the transport coefficients were calculated (in the 13M-approximation) for large aspect ratio tokamaks in the limit of low collision frequency employing the small mass-ratio approximation for the unlike-species collision term C_{ab} [60].

The averaged radial electron flux, the averaged radial electron heat flux as well as the average of the parallel current density were written as

$$\Gamma_e = \sum_{n=1}^{4} (\alpha_1, g_{ne}) A_{ne}$$
 (7.95)

$$\frac{q_e}{T_e} = \sum_{n=1}^{4} (\alpha_2, g_{ne}) A_{ne}$$
 (7.96)

$$\frac{1}{T_e} \left\langle \frac{J_{\parallel} - J_{\parallel s}}{h} \right\rangle = \sum_{n=1}^{4} (\alpha_3, g_{ne}) A_{ne}, \tag{7.97}$$

where

$$J_{\parallel s} \equiv \sigma_{\parallel} B \frac{\langle E_{\parallel} B \rangle}{\langle B^2 \rangle} \tag{7.98}$$

defines the Spitzer current density and $h=B_0^{\rm HH}/B$. The thermodynamic forces were defined as follows

$$A_{1e} = \frac{\partial}{\partial \rho} \ln p_e + \frac{T_i}{Z_i T_e} \frac{\partial}{\partial \rho} \ln p_i \tag{7.99}$$

$$A_{2e} = \frac{\partial}{\partial \varrho} \ln T_e \tag{7.100}$$

$$A_{3e} = B_0^{\text{HH}} \frac{\langle E_{\parallel} B \rangle}{\langle B^2 \rangle}, \tag{7.101}$$

with ϱ being the effective minor radius coordinate which reduces to the usual minor radius r in the large aspect ratio, circular cross section case [60]. The inner products

$$(\alpha_m, g_{ne}) = \left\langle \int d^3 v \alpha_m g_{ne} \right\rangle, \quad \text{for} \quad m, n = 1, 2, 3$$
 (7.102)

are the electron transport coefficients,

$$(\alpha_m, g_{ne}) = K_{mn}^b \epsilon^{1/2} \frac{n_e \rho_{e\theta}^2}{\tau_e}, \quad \text{for} \quad m, n = 1, 2 \quad (7.103)$$

$$(\alpha_m, g_{3e}) = (\alpha_3, g_{me}) = K_{m3}^b \epsilon^{1/2} \frac{n_e c}{B_{p0}}, \quad \text{for } m = 1, 2$$
 (7.104)

$$(\alpha_3, g_{3e}) = K_{33}^b \epsilon^{1/2} \frac{\sigma_{\parallel}}{T_e}, \tag{7.105}$$

satisfying the Onsager symmetry $(\alpha_m, g_{ne}) = (\alpha_n, g_{me})$ and where the set of dimensionless banana regime (that is the collisionality parameter $\nu_* \to 0$) transport coefficients are functions of ion charge,

$$K_{11}^b = -0.73 \left(1 + \frac{0.53}{Z_i} \right) \tag{7.106}$$

$$K_{12}^b = 1.10 \left(1 + \frac{0.41}{Z_i} \right) \tag{7.107}$$

$$K_{22}^b = -2.37 \left(1 + \frac{0.43}{Z_i} \right) \tag{7.108}$$

$$K_{13}^b = -1.46 \left(1 + \frac{0.67}{Z_i} \right) \tag{7.109}$$

$$K_{23}^b = \frac{1.75}{Z_i} (7.110)$$

$$K_{33}^b = -1.46 \left(1 + \frac{0.34}{Z_i} \right).$$
 (7.111)

The Z_i dependence is an approximate fit based on the $Z_i = 1$ and $Z_i \to \infty$ results [60]. An approximate analytical expression for the Z_i dependence of the parallel conductivity is

$$\sigma_{\parallel} = \frac{n_e e^2 \tau_e}{m_e} \left(0.29 + \frac{0.46}{1.08 + Z_i} \right)^{-1}.$$
 (7.112)

Here,

$$\tau_e = \frac{3}{16\sqrt{\pi}} \frac{v_{te}^3 m_e^2}{n_i Z_i^2 e^4 \ln \Lambda},\tag{7.113}$$

is the electron collision time, $B_{p0} \equiv B_0^{\rm HH}/(R_0B_{T0})\partial\chi/\partial r$ is the effective poloidal field magnitude and $\rho_{e\theta}^2 \equiv v_{te}^2/\Omega_{ep}^2 = 2m_ec^2T_e/(e^2B_{p0}^2)$, where χ is the poloidal flux, B_{T0} is a representative value of the toroidal magnetic field and $B_0^{\rm HH}$ is an arbitrarily chosen function normalizing the magnetic field. In the case of the standard tokamak test configuration (cf. Appendix F) B_{T0} has been chosen to be \mathcal{B}_0 from which it follows that $B_{p0} = \iota \epsilon B_0^{\rm HH}$, where $\iota = \mathrm{d}\chi/\mathrm{d}\psi$, $\partial\psi/\partial r = \mathcal{B}_0 r$ and $\epsilon = r/R_0$ has been used.

Recalling Eq. (7.6) the dimensionless diffusion coefficients may be expressed as

$$\gamma_{mn}^{'\mathrm{HH}} = -\frac{\tau_{ee}}{n_e} \frac{(\alpha_m, g_{ne})}{\rho^2}$$

$$= -\frac{\tau_{ee}}{\tau_e} \frac{\rho_{e\theta}^2}{\rho^2} \epsilon^{1/2} K_{mn}^b(Z_{\text{eff}})$$

$$= -\frac{Z_{\text{eff}}}{\epsilon^2 \epsilon^{3/2}} K_{mn}^b(Z_{\text{eff}}), \qquad (7.114)$$

valid for m, n = 1, 2. Here, τ_{ee}/τ_e has been replaced by Z_{eff} and

$$\frac{\rho_{e\theta}^2}{\rho^2} = \frac{b_0^2}{B_{p0}^2} = \frac{1}{t^2 \epsilon^2},\tag{7.115}$$

where $B_0^{\rm HH}=B_0=b_0$ has been utilized. Making use of the fact that $A_{3e}=-B_0^{\rm HH}T_e/(B_0e)A_3$ leads to

$$\gamma_{m3}^{'\text{HH}} = \gamma_{3m}^{'\text{HH}} = \frac{\tau_{ee}}{n_e \rho l_c} \frac{B_0^{\text{HH}}}{B_0} \frac{T_e}{e} (\alpha_m, g_{3e})
= \frac{\sqrt{\epsilon}}{2} \frac{B_0^{\text{HH}}}{B_{p0}} K_{m3}^b (Z_{\text{eff}})
= \frac{K_{m3}^b (Z_{\text{eff}})}{2t\sqrt{\epsilon}}, \quad \text{for } m = 1, 2.$$
(7.116)

A comparison between Eqs. (7.97) and (7.101) as well as Eqs. (7.2) and (7.5) yields the dimensionless conductivity coefficient

$$\gamma_{33}^{'\text{HH}} = -\frac{\tau_{ee}}{n_e l_c^2} \left[\frac{T_e^2}{e^2} \left(\frac{B_0^{\text{HH}}}{B_0} \right)^2 (\alpha_3, g_{3e}) + \frac{T_e}{e^2} \sigma_{\parallel} \langle \hat{B}^2 \rangle \right] \\
= -\frac{T_e \sigma_{\parallel}}{e^2} \left[\left(\frac{B_0^{\text{HH}}}{B_0} \right)^2 \sqrt{\epsilon} K_{33}^b (Z_{\text{eff}}) + \langle \hat{B}^2 \rangle \right] \\
= -\frac{1}{2Z_{\text{eff}} K_{\parallel} (Z_{\text{eff}})} \left[\sqrt{\epsilon} K_{33}^b (Z_{\text{eff}}) + \langle \hat{B}^2 \rangle \right],$$
(7.117)

where K_{\parallel} corresponds to the bracketed denominator in Eq. (7.112). Finally, to obtain the desired banana regime transport coefficients $\gamma_{mn}^{\rm HH}$, the $\gamma_{mn}^{'\rm HH}$ matrix has to be transformed as described at the end of Chapter 7.1 [see Eqs. (7.50)-(7.55)].

Hinton and Hazeltine also presented an approximate analytical representation for the transport coefficients expressing them as continuous functions of collisionality [60]. The results were obtained by least-squares fits to the following functions

$$K_{mn} = K_{mn}^{(0)} \left[\frac{1}{1 + a_{mn}\sqrt{\nu_{*e}} + b_{mn}\nu_{*e}} + \frac{\epsilon^{3/2}c_{mn}^2\nu_{*e}\epsilon^{3/2}}{b_{mn}(1 + c_{mn}\nu_{*e}\epsilon^{3/2})} \right], \quad (7.118)$$

valid for m or n = 1 or 2 and

$$K_{m3} = K_{m3}^{(0)} \left[\frac{1}{(1 + a_{m3}\sqrt{\nu_{*e}} + b_{m3}\nu_{*e})(1 + c_{m3}\nu_{*e}\epsilon^{3/2})} \right], \tag{7.119}$$

for n=3, respectively, and where ν_{*e} represents the electron collisionality parameter

$$\nu_{*e} \equiv \frac{\sqrt{2}rB_0^{\rm HH}}{B_{v0}v_{te}\tau_e\epsilon^{3/2}} = \frac{\sqrt{2}R_0Z_{\rm eff}}{\iota v_{te}\tau_{ee}\epsilon^{3/2}}.$$
 (7.120)

The values for the numerical coefficients $K_{mn}^{(0)}(Z_i)$, $a_{mn}(Z_i)$, $b_{mn}(Z_i)$ and $c_{mn}(Z_i)$ are listed in Table III of Reference 60 for $Z_i = 1, 2$ and 4. It has to be noted that the coefficients $K_{mn}^{(0)}$ do not exactly agree with the banana regime (where ν_{*e} tends to zero) values K_{mn}^{b} since they were calculated from least-squares fits [60].

The electron transport coefficients have been defined as follows

$$-(\alpha_1, g_{1e}) = K_{11} \epsilon^{1/2} \frac{n_e \rho_{e\theta}^2}{\tau_e}$$
 (7.121)

$$-(\alpha_1, g_{2e}) - \frac{5}{2}(\alpha_1, g_{1e}) = K_{12} \epsilon^{1/2} \frac{n_e \rho_{e\theta}^2}{\tau_e}$$
 (7.122)

$$-(\alpha_2, g_{1e}) - 5(\alpha_1, g_{2e}) - \frac{25}{4} - (\alpha_1, g_{1e}) = K_{22} \epsilon^{1/2} \frac{n_e \rho_{e\theta}^2}{\tau_e}$$
 (7.123)

$$-(\alpha_1, g_{3e}) = K_{13} \epsilon^{1/2} \frac{n_e c}{B_{p0}}$$
 (7.124)

$$-(\alpha_2, g_{3e}) - \frac{5}{2}(\alpha_1, g_{3e}) = K_{23} \epsilon^{1/2} \frac{n_e c}{B_{p0}}$$
 (7.125)

$$-(\alpha_3, g_{3e}) = K_{33} \epsilon^{1/2} \frac{\sigma_{\parallel}}{T_e}$$
 (7.126)

from which one may derive that

$$\gamma_{mn}^{\text{HH}} = \frac{Z_{\text{eff}}}{t^2 \epsilon^{3/2}} K_{mn}(\epsilon, Z_{\text{eff}}, \nu_{*e}), \quad \text{for} \quad m, n = 1, 2,$$
(7.127)

and

$$\gamma_{m3}^{\text{HH}} = -\frac{K_{m3}(\epsilon, Z_{\text{eff}}, \nu_{*e})}{2t\sqrt{\epsilon}}, \quad \text{for} \quad m = 1, 2,$$
(7.128)

respectively. The transport coefficient representing the electrical conductivity reads

$$\gamma_{33}^{\text{HH}} = \frac{1}{2Z_{\text{eff}}K_{\parallel}(Z_{\text{eff}})} \left[\sqrt{\epsilon} K_{33}(\epsilon, Z_{\text{eff}}, \nu_{*e}) - \left\langle \hat{B}^2 \right\rangle \right]. \tag{7.129}$$

Equations (7.127)-(7.129) have to be compared with the NEO-2 results.

In Reference 66 finite aspect ratio modifications to the neoclassical transport coefficients L_{mn} (for $Z_i = 1$) in the limit of small collision frequency were obtained by a combination of large and small aspect ratio limit results. The coefficients are not in general exact and are restricted to the case of nearly concentric circular flux surfaces. The elements of the transport matrix are

$$L_{11}^{\text{\tiny HHm}} = \frac{n_e}{\tau_e} \rho_{e\theta}^2 \left(1.12\sqrt{\epsilon} - 0.62\epsilon \right) \tag{7.130}$$

$$L_{12}^{\text{\tiny HHm}} = \frac{n_e}{\tau_e} \rho_{e\theta}^2 \left(1.27\sqrt{\epsilon} - 0.77\epsilon \right) \tag{7.131}$$

$$L_{22}^{\text{HHm}} = \frac{n_e}{\tau_e} \rho_{e\theta}^2 \left(2.64 \sqrt{\epsilon} - 0.933 \epsilon \right)$$
 (7.132)

$$L_{22}^{\text{HHm}} = \frac{n_e}{\tau_e} \rho_{e\theta}^2 \left(2.64 \sqrt{\epsilon} - 0.933 \epsilon \right)$$

$$L_{13}^{\text{HHm}} = \frac{cn_e}{B_{p0}} \left(2.44 \sqrt{\epsilon} - 1.44 \epsilon \right)$$
(7.132)

$$L_{23}^{\text{HHm}} = \frac{\dot{cn_e}}{B_{p0}} \left(4.35\sqrt{\epsilon} - 1.85\epsilon \right)$$
 (7.134)

$$L_{33}^{\text{\tiny HHm}} = \frac{\sigma_{\parallel}}{T_e} \left(1.95\sqrt{\epsilon} - 0.950\epsilon \right), \tag{7.135}$$

where the $\mathcal{O}(\sqrt{\epsilon})$ -terms correspond to the $\nu_{*e} \to 0$ limit presented above. Thus, the dimensionless modified transport coefficients become

$$\gamma_{11}^{\text{HHm}} = \gamma_{11}^{\text{HH}}(Z_{\text{eff}} = 1) - \frac{0.62}{t^2 \epsilon}$$
(7.136)

$$\gamma_{12}^{\text{\tiny HHm}} = \gamma_{12}^{\text{\tiny HH}}(Z_{\text{eff}} = 1) - \frac{0.77}{t^2 \epsilon}$$
(7.137)

$$\gamma_{22}^{\text{HHm}} = \gamma_{22}^{\text{HH}}(Z_{\text{eff}} = 1) - \frac{0.933}{t^2 \epsilon}$$
(7.138)

$$\gamma_{13}^{\text{HHm}} = \gamma_{13}^{\text{HH}}(Z_{\text{eff}} = 1) + \frac{1.44}{2t}$$
(7.139)

$$\gamma_{23}^{\text{HHm}} = \gamma_{23}^{\text{HH}}(Z_{\text{eff}} = 1) + \frac{1.85}{2t}$$

$$\gamma_{33}^{\text{HHm}} = \gamma_{33}^{\text{HH}}(Z_{\text{eff}} = 1) - \frac{0.95\epsilon}{2K_{\parallel}(1)}.$$
(7.140)

$$\gamma_{33}^{\text{HHm}} = \gamma_{33}^{\text{HH}}(Z_{\text{eff}} = 1) - \frac{0.95\epsilon}{2K_{\parallel}(1)}.$$
(7.141)

Sauter-Angioni 7.4

In References 38,61 (see also [62,63]) the neoclassical transport coefficients have been calculated for general axisymmetric equilibria and arbitrary collisionality regime applying the full linearized collision operator. Their expressions have been obtained by solving numerically the Fokker-Planck equation (using an adjoint function formalism [67,68]) varying the trapped particle fraction, the collisionality parameter and the effective ion charge. Finally, a set of

formulas representing the transport coefficients has been proposed fitting these code results.

The expressions which relate the thermodynamic fluxes to forces have been written as

$$I_m = \sum_{n=1}^{3} \mathcal{L}_{mn}^e \mathcal{A}_{en}, \quad \text{for} \quad m = 1, 2, 3,$$
 (7.142)

where

$$I_1 \equiv \Gamma_e \frac{\mathrm{d}\chi}{\mathrm{d}\varrho}, \qquad I_2 \equiv \frac{q_e}{T_e} \frac{\mathrm{d}\chi}{\mathrm{d}\varrho},$$
 (7.143)

and

$$I_3 \equiv \left\langle \frac{j_{\parallel}B}{T_e} \right\rangle - \left\langle \frac{j_{\parallel s}B}{T_e} \right\rangle, \tag{7.144}$$

respectively. Here, Γ_e and q_e are the perpendicular electron particle and heat fluxes, j_{\parallel} is the total parallel electric current, $j_{\parallel s}$ is the Spitzer current and \mathcal{A}_{en} are the driving forces,

$$\mathcal{A}_{e1}(\chi) = \frac{1}{p_e} \frac{\mathrm{d}p_e}{\mathrm{d}\chi} + \frac{1}{p_e} \frac{\mathrm{d}p_i}{\mathrm{d}\chi}$$
 (7.145)

$$\mathcal{A}_{e2}(\chi) = \frac{1}{T_e} \frac{\mathrm{d}T_e}{\mathrm{d}\chi}$$
 (7.146)

$$\mathcal{A}_{e3}(\chi) = \frac{\langle E_{\parallel} B \rangle}{\langle B^2 \rangle}. \tag{7.147}$$

The driving force \mathcal{A}_{e3} can be expressed in terms of A_3 [cf. Eq. (7.5)] yielding $\mathcal{A}_{e3} = -A_3T_e/(eB_0)$. The elements of the transport matrix satisfy the Onsager symmetry, that is $\mathcal{L}_{mn}^e = \mathcal{L}_{nm}^e$.

The diffusive transport coefficients in the low collisionality limit ($\nu_{e*} \to 0$) have been defined as follows [38]

$$\mathcal{L}_{mn}^{e} = \frac{n_e \rho_{ep}^2}{\tau_e} \left(\frac{\mathrm{d}\chi}{\mathrm{d}\varrho}\right)^2 (B_0^{\mathrm{AS}})^2 \langle B^{-2} \rangle \mathcal{K}_{mn}^{e}(f_t^d), \tag{7.148}$$

for m, n = 1, 2, where

$$\tau_e = \frac{3}{16\sqrt{\pi}} \frac{v_{te}^3 m_e^2}{n_i Z_i^2 e^4 \ln \Lambda},\tag{7.149}$$

 $ho_{ep}^2 = v_{te}^2/\Omega_{ep}^2 = 2T_e m_e c^2/(e^2 B_{p0}^2)$ is the square of the poloidal gyroradius, $B_{p0} = [B_0^{\rm AS}(\chi)/I(\chi)](\mathrm{d}\chi/\mathrm{d}\varrho)$ is the poloidal magnetic field, $B_0^{\rm AS}$ is an arbitrarily chosen function normalizing the magnetic field, χ is the poloidal flux

and \mathcal{K}_{mn}^{e} represents the dimensionless electron transport coefficients in the banana regime,

$$\mathcal{K}_{11}^e(f_t^d) = -0.5F_{11}(f_t^d) \tag{7.150}$$

$$\mathcal{K}_{12}^{e}(f_t^d) = 0.75F_{12}(f_t^d) \tag{7.151}$$

$$\mathcal{K}_{22}^{e}(f_t^d) = -\left(\frac{13}{8} + \frac{\sqrt{2}}{2Z}\right) F_{22}(f_t^d),$$
 (7.152)

with

$$F_{11}(X) \equiv \left(1 + \frac{0.9}{Z + 0.5}\right) X - \frac{1.9X^2}{Z + 0.5} + \frac{1.6X^3}{Z + 0.5} - \frac{0.6X^4}{Z + 0.5}$$
 (7.153)

$$F_{12}(X) \equiv \left(1 + \frac{0.6}{Z + 0.5}\right) X - \frac{0.95X^2}{Z + 0.5} + \frac{0.3X^3}{Z + 0.5} + \frac{0.05X^4}{Z + 0.5}$$
 (7.154)

$$F_{22}(X) \equiv \left(1 - \frac{0.11}{Z + 0.5}\right) X + \frac{0.08X^2}{Z + 0.5} + \frac{0.03X^3}{Z + 0.5}$$
 (7.155)

and

$$f_t^d = 1 - \frac{1 - f_t}{\langle B^2 \rangle \langle B^{-2} \rangle},$$
 (7.156)

with f_t being the trapped particle fraction. For the standard tokamak test configuration defined in Appendix F.3.2 the function f_t is approximated using Eq. (7.26). Here, $B_0^{\text{AS}} \equiv B_0 = b_0$ is assumed producing the averaged quantities $\langle \hat{B}^2 \rangle = (1 - \epsilon^2)^{3/2}$ and $\langle \hat{B}^{-2} \rangle = (2 + 3\epsilon^2)/[2(1 - \epsilon^2)^2]$, respectively. Thus,

$$f_t^d = 1 - \frac{2\sqrt{1 - \epsilon^2}}{2 + 3\epsilon^2} (1 - f_t). \tag{7.157}$$

The function I corresponds to the quantity J in Appendix F [see Eq. (F.45)]. After applying $d/d\chi = (1/t)d/d\psi$, $\langle |\nabla \psi| \rangle d/d\psi \equiv d/dr$, $\varrho \equiv r$, using Eqs. (7.1)-(7.5) and by means of

$$I_m(r) = \frac{\mathcal{L}_{m1}^e}{t^2 \langle |\nabla \psi| \rangle^2} \mathcal{A}_{e1}(r) + \frac{\mathcal{L}_{m2}^e}{t^2 \langle |\nabla \psi| \rangle^2} \mathcal{A}_{e2}(r) + \frac{\mathcal{L}_{m3}^e}{t \langle |\nabla \psi| \rangle} \mathcal{A}_{e3}(r), \qquad (7.158)$$

for m = 1, 2 one may infer that

$$\gamma_{mn}^{'e, AS} = -\frac{\tau_{ee}}{n_e \rho^2} \frac{\mathcal{L}_{mn}^e}{t^2 \langle |\nabla \psi| \rangle^2}, \tag{7.159}$$

from which it follows that, by substituting Eq. (7.148),

$$\gamma_{mn}^{'e, AS} = -\frac{\tau_{ee}}{\tau_e} \left(\frac{\rho_{ep}}{\rho}\right)^2 \langle \hat{B}^{-2} \rangle K_{mn}^e(f_t^d). \tag{7.160}$$

The ratio of the collision times has to be replaced by Z_{eff} , and the ratio of the Larmor radii reads

$$\left(\frac{\rho_{ep}}{\rho}\right)^2 = \frac{b_0^2}{B_{p0}^2} = \frac{1 - \epsilon^2}{\epsilon^2 \epsilon^2},\tag{7.161}$$

where, for the standard tokamak case,

$$B_{p0} = \iota \frac{\mathrm{d}\psi}{\mathrm{d}r} \frac{b_0}{J} = \frac{\iota \epsilon}{\sqrt{1 - \epsilon^2}} b_0, \tag{7.162}$$

has been substituted (noting that $J = \mathcal{B}_0 R_0 \sqrt{1 - \epsilon^2}$). Therefore, the diffusion coefficients in the collisionless limit become

$$\gamma_{mn}^{'e,AS} = -\frac{Z_{\text{eff}}}{t^2} \frac{(2+3\epsilon^2)}{2\epsilon^2(1-\epsilon^2)} \mathcal{K}_{mn}^e(f_t^d), \quad \text{for} \quad m, n = 1, 2.$$
 (7.163)

For arbitrary collisionality regimes Angioni and Sauter proposed for the dimensionless transport coefficients the following expressions [38]

$$\mathcal{K}_{11}^{e}(f_{t}^{d}, \nu_{e*}) = \mathcal{H}_{11}^{e} \tag{7.164}$$

$$\mathcal{K}_{12}^{e}(f_{t}^{d}, \nu_{e*}) = \mathcal{H}_{12}^{e} - \frac{5}{2}\mathcal{H}_{11}^{e}$$
 (7.165)

$$\mathcal{K}_{22}^{e}(f_{t}^{d}, \nu_{e*}) = \mathcal{H}_{22}^{e} - 5\mathcal{H}_{12}^{e} + \frac{25}{4}\mathcal{H}_{11}^{e},$$
 (7.166)

with

$$\mathcal{H}_{mn}^{e}(f_{t}^{d}, \nu_{e*}) = \frac{\mathcal{H}_{mn}^{e(0)}(f_{t}^{d}, \nu_{e*} = 0)}{1 + a_{mn}(Z)\sqrt{\nu_{ef*}} + b_{mn}(Z)\nu_{ef*}} - \frac{d_{mn}(Z)(f_{t}^{d})^{3}[1 + (f_{t}^{d})^{6}]\nu_{ef*}}{1 + c_{mn}(Z)(f_{t}^{d})^{3}[1 + (f_{t}^{d})^{6}]\nu_{ef*}} F_{PS}, \quad (7.167)$$

where $F_{PS} = 1 - 1/(\langle B^2 \rangle \langle B^{-2} \rangle)$, the collisionality parameter

$$\nu_{e*} = 6.921 \cdot 10^{-18} \frac{qRn_e Z_{\text{eff}} \ln \Lambda_e}{T_e^2 \epsilon^{3/2}}, \tag{7.168}$$

where q is the safety factor, the density is given in m⁻³ and the temperature in eV, respectively and $\nu_{ef*} = \nu_{e*}/(1+7f_t^2)$ is a rescaled collisionality parameter. Here, Eq. (7.168) may be converted to

$$\nu_{e*} = \frac{\sqrt{2}R_0 Z_{\text{eff}}}{\iota v_{te} \tau_{ee} \epsilon^{3/2}}.$$
 (7.169)

The coefficients $\mathcal{H}_{mn}^{e(0)}$ for m, n = 1, 2 are given by

$$\mathcal{H}_{11}^{e(0)} = \mathcal{K}_{11}^{e}(f_t^d) \tag{7.170}$$

$$\mathcal{H}_{12}^{e(0)} = \mathcal{K}_{12}^{e}(f_t^d) + \frac{5}{2}\mathcal{K}_{11}^{e}(f_t^d)$$
 (7.171)

$$\mathcal{H}_{22}^{e(0)} = \mathcal{K}_{22}^{e}(f_t^d) + 5\mathcal{K}_{12}^{e}(f_t^d) + \frac{25}{4}\mathcal{K}_{11}^{e}(f_t^d), \tag{7.172}$$

where the functions $a_{mn}(Z)$, $b_{mn}(Z)$, $c_{mn}(Z)$ and $d_{mn}(Z)$ can be found in Appendix B of Reference 38.

The calculation of the neoclassical conductivity and the bootstrap current has been presented in Reference 61 where the flux surface averaged total parallel current has been given by the relation

$$\langle j_{\parallel}B\rangle = \sigma_{\text{neo}}\langle E_{\parallel}B\rangle - I(\chi)p_e \left[\mathcal{L}_{31}^e \mathcal{A}_{e1}(\chi) + \mathcal{L}_{32}^e \mathcal{A}_{e2}(\chi)\right], \tag{7.173}$$

which can be rewritten as

$$-\frac{1}{e}\langle j_{\parallel}\hat{B}\rangle = \frac{\sigma_{\text{neo}}T_{e}}{e^{2}}\langle \hat{B}^{2}\rangle A_{3}(r) + \frac{In_{e}T_{e}}{eB_{0}t\langle|\nabla\psi|\rangle} \left[\mathcal{L}_{31}^{e}\mathcal{A}_{e1}(r) + \mathcal{L}_{32}^{e}\mathcal{A}_{e2}(r)\right], \qquad (7.174)$$

yielding the dimensionless electron transport coefficients

$$\gamma_{3n}^{'AS} = -\frac{\tau_{ee}}{n_e l_c \rho} \frac{I n_e T_e}{e B_0 t \langle |\nabla \psi| \rangle} \mathcal{L}_{3n}^e
= -\frac{J}{2t \langle |\nabla \psi| \rangle} \mathcal{L}_{3n}^e
= -\frac{\sqrt{1 - \epsilon^2}}{2t \epsilon} \mathcal{L}_{3n}^e, \quad \text{for} \quad n = 1, 2,$$
(7.175)

as well as

$$\gamma_{33}^{'AS} = -\frac{\tau_{ee}}{n_e l_c^2} \frac{\sigma_{\text{neo}} T_e}{e^2} \langle \hat{B}^2 \rangle$$

$$= -\frac{\sigma_{\text{Sp}} \langle \hat{B}^2 \rangle T_e m_e}{n_e e^2 \tau_{ee} 2 T_e} \frac{\sigma_{\text{neo}}}{\sigma_{\text{Sp}}}$$

$$= -\frac{1.96}{2} \frac{\langle \hat{B}^2 \rangle}{Z_{\text{eff}} N(Z_{\text{eff}})} \frac{\sigma_{\text{neo}}}{\sigma_{\text{Sp}}}, \tag{7.176}$$

where

$$\sigma_{\rm Sp} = 1.9012 \cdot 10^4 \frac{T_e [{\rm eV}]^{3/2}}{Z_{\rm eff} N(Z_{\rm eff}) \ln \Lambda_e} [{\rm m}^{-1} \Omega^{-1}]$$
 (7.177)

$$= 1.96 \frac{n_e e^2 \tau_{ee}}{Z_{\text{eff}} N(Z_{\text{eff}}) m_e}, \tag{7.178}$$

and N(Z) = 0.58 + 0.74/(0.76 + Z) has been applied, respectively. The functions \mathcal{L}_{3n}^e and the ratio $\sigma_{\text{neo}}/\sigma_{\text{Sp}}$ represent analytical fits to code results (for details see Reference 61) and have the following form

$$\mathcal{L}_{31}^{e} = F_{31}(X = f_{\text{teff}}^{31}) \equiv \left(1 + \frac{1.4}{Z+1}\right) X - \frac{1.9}{Z+1} X^{2} + \frac{0.3}{Z+1} X^{3} + \frac{0.2}{Z+1} X^{4}, \tag{7.179}$$

$$\mathcal{L}_{32}^{e} = F_{32_ee}(X = f_{\text{teff}}^{32_ee}) + F_{32_ei}(Y = f_{\text{teff}}^{32_ei}), \tag{7.180}$$

with

$$F_{32_ee}(X) = \frac{0.05 + 0.62Z}{Z(1 + 0.44Z)}(X - X^4) + \frac{X^2 - X^4 - 1.2(X^3 - X^4)}{1 + 0.22Z} + \frac{1.2}{1 + 0.5Z}X^4$$

$$F_{32_ei}(Y) = -\frac{0.56 + 1.93Z}{Z(1 + 0.44Z)}(Y - Y^4) + \frac{4.95[Y^2 - Y^4 - 0.55(Y^3 - Y^4)]}{1 + 2.48Z} - \frac{1.2}{1 + 0.5Z}Y^4,$$

$$(7.182)$$

and

$$\frac{\sigma_{\text{neo}}}{\sigma_{\text{Sp}}} = F_{33}(X = f_{\text{teff}}^{33}) \equiv 1 - \left(1 + \frac{0.36}{Z}\right)X + \frac{0.59}{Z}X^2 - \frac{0.23}{Z}X^3, \quad (7.183)$$

as well as

$$f_{\text{teff}}^{33}(\nu_{e*}) = \frac{f_t}{1 + (0.55 - 0.1f_t)\sqrt{\nu_{e*}} + 0.45(1 - f_t)\nu_{e*}/Z_{\text{off}}^{3/2}}$$
(7.184)

$$f_{\text{teff}}^{31}(\nu_{e*}) = \frac{f_t}{1 + (1 - 0.1 f_t) \sqrt{\nu_{e*}} + 0.5(1 - f_t) \nu_{e*} / Z_{\text{eff}}}$$
(7.185)

$$f_{\text{teff}}^{32\text{_}ee}(\nu_{e*}) = \frac{f_t}{1 + 0.26(1 - f_t)\sqrt{\nu_{e*}} + 0.18(1 - 0.37f_t)\nu_{e*}/\sqrt{Z_{\text{eff}}}}$$
(7.186)

$$f_{\text{teff}}^{32_ei}(\nu_{e*}) = \frac{f_t}{1 + (1 + 0.6f_t)\sqrt{\nu_{e*}} + 0.85(1 - 0.37f_t)\nu_{e*}(1 + Z_{\text{eff}})}.$$
 (7.187)

In the collisionless limit ($\nu_{e*} \to 0$), these functions reduce to the trapped particle fraction f_t [61], that is $f_{\text{teff}}^{31} = f_{\text{teff}}^{32_ee} = f_{\text{teff}}^{32_ei} = f_{\text{teff}}^{33} = f_t$. Finally, the transport matrix to be compared with NEO-2 results is obtained upon a transformation according to Eqs. (7.50)-(7.55).

7.5 Numerical results

In this section, the dimensionless electron transport coefficients γ_{jk} are calculated for a large aspect ratio tokamak ($\epsilon = 0.05$ and $\epsilon = 0.52$) with concentric circular flux surfaces (see Appendix F).

The numerical values of the transport coefficients obtained from the analytical models presented in the previous sections are valid in the collisionless limit $(\nu_{e*} \to 0)$ and for $Z_{\rm eff} = 1$ and are collected in Table 7.1 together with the NEO-2 results. The NEO-2 results have been evaluated at the collisionality $L_c/l_c \equiv 2\pi R_0/(v_{te}\tau_{ee}) = 10^{-8}$ using five Laguerre and four Legendre polynomials, respectively. The computation accuracy of the transport coefficients improves with both, grid resolution and (mainly) number of Laguerre polynomials in modeling energy dependence.

Table 7.1: Transport matrix γ_{jk}^e in the collisionless limit: NEO-2 results vs. analytical results presented in the literature (for $Z_{\text{eff}} = 1$)

	NEO-2	Bal	Hir	НН	$\mathrm{HH}_{\mathrm{mod}}$	SA
γ_{11}	366.56	311.74	310.48	370.06	324.20	312.15
γ_{12}	304.12	337.17	337.17	413.59	356.64	337.85
γ_{21}	340.31	337.17	337.17	413.59	356.64	337.85
γ_{22}	839.48	805.78	829.66	879.18	810.17	809.04
$-\gamma_{13}$	8.56	8.54		10.50	9.12	8.75
$-\gamma_{31}$	8.56	8.54	8.52	10.50	9.12	8.75
$-\gamma_{23}$	17.13	16.55		18.73	16.95	17.56
$-\gamma_{32}$	16.97	16.55	16.46	18.73	16.95	17.56
$-\gamma_{33}$	0.613	0.615	0.614	0.547	0.593	0.600

The NEO-2 results for the transport matrix are in very reasonable agreement with results calculated by the formulas given in previous sections. The main differences arise from the collision operator (Balescu, Hirshman) as well as from using large aspect ratio expressions (Hinton and Hazeltine) and, respectively, from the fact that the results have been fitted with respect to

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trapped particle fraction (that is to the aspect ratio), collisionality parameter and effective charge (Sauter et al.).

The results for the transport coefficients as a function of the collisionality parameter L_c/l_c and for the effective charge number $Z_{\text{eff}} = 1, 2$ and 4 are shown in Chapter 8 (see Figures 8.1-8.6) noting that the relation between the collisionality parameters is given by

$$\nu_{e*} = \frac{\sqrt{2}R_0 Z_{\text{eff}}}{\iota v_{te} \tau_{ee} \epsilon^{3/2}} = \frac{Z_{\text{eff}}}{\sqrt{2}\pi \iota \epsilon^{3/2}} \frac{L_c}{l_c}.$$
 (7.188)

Chapter 8

Computational results for a standard tokamak

In this chapter the computational results for a standard tokamak with circular cross section (see Appendix F) obtained by the NEO-2 code are presented. It has to be noted that these results have meanwhile been published in the following refereed journal articles:

- Recent progress in NEO-2 A code for neoclassical transport computations based on field line tracing
 W. Kernbichler, S. V. Kasilov, G. O. Leitold, V. V. Nemov and K. Allmaier, Plasma and Fusion Research 3, S1061 (2008)
- Generalized Spitzer Function with Finite Collisionality in Toroidal Plasmas

W. Kernbichler, S. V. Kasilov, G. O. Leitold, V. V. Nemov and N. B. Marushchenko, Contrib. Plasma Phys. **50**, 761 (2010)

The neoclassical electron transport coefficients are compared to the analytical results in the axisymmetric limit obtained by Hinton and Hazeltine and by Angioni and Sauter, respectively. The Hinton-Hazeltine results have been calculated using a small mass-ratio approximation for the unlike-species collision operator and are valid for large aspect ratio and all collisionalities [60] whereas the Angioni-Sauter results have been computed for all aspect ratios and collisionalities applying a full linearized collision operator [38,61]. Furthermore, the generalized Spitzer function taking into account finite plasma collisionality is computed by NEO-2 and is compared to the collisionless approximation computed by the SYNCH code [69].

At the beginning the drift kinetic equation (DKE) solver NEO-2 is briefly described.

8.1 NEO-2 code

The code NEO-2 is a solver for the DKE in the case of negligible small $\mathbf{E} \times \mathbf{B}$ drift which is based on the method of field line tracing. Originally, it was developed to compute monoenergetic transport coefficients (that is, only the Lorentz collision operator was implemented) with the special aim of good convergence in low collisionality regimes. This is accomplished through adaptive level placement over the normalized magnetic moment η . With this adaptive placement NEO-2 effectively resolves steep behavior of the distribution function f at the trapped passing boundary. In this context NEO-2 has been extensively benchmarked with DKES [70,71] and various Monte Carlo codes [26,72,73].

In addition, NEO-2 can also use the full linearized collision operator including energy diffusion and momentum conserving integral response of the background particles. This has been managed by a transformation of DKE to a set of coupled ordinary differential equations (see Chapter 3.1) with respect to the parallel variable (distance counted along the field line) presenting energy dependence of the distribution function in the form of an expansion over associated Laguerre polynomials and discretizing dependence of the expansion coefficients on the normalized magnetic moment on the adaptive non-equidistant grid.

In NEO-2 the perpendicular (cross field) rotation of the plasma within the flux surface (which is mainly in the poloidal direction), in particular the rotation due to the radial electric field is ignored in the DKE. This limits its usage in the computation of neoclassical transport data base entries for monoenergetic transport coefficients. For ECCD computations, however, radial electric fields play practically no role and therefore NEO-2 is not limited to certain regimes. At the moment, a non-relativistic collision operator is used, but this is not an intrinsic limitation and can be improved during further development.

Presently, the main limitation is the speed of the code which restricts practical usage to tokamak problems. This limitation is caused by the stiffness of the ODE set resulting from the discretization of the DKE over normalized magnetic moment η and momentum module. Namely, the usual Runge-Kutta ODE solver used up to now in NEO-2 needs an extremely small integration step along the field line which is orders of magnitude smaller than the scale of the solution. Partly such stiffness is present already in mono-energetic computations due to the η -grid refinement in the trapped-passing boundary layer (and transition layers between different classes of trapped particles in the case of stellarators). This stiffness significantly increases in computations with the full linearized collision operator because there one formally has to solve simultaneously the problem for different energies (and, respectively,

different collisionalities) using the same grid over η which results in excessive grid density for low energies. This technical problem should be resolved in future with implementation of an exponential integrator instead of the usual ODE solver. An additional independent possibility to speed up the computations is parallelization of the code. A parallel version of the code is possible since the DKE is actually solved in NEO-2 on portions of the field line (propagators) which are treated independently from each other and can be distributed between the processors. Such independent solutions are then linked together at the very end of the computation giving the final solution. These improvements should make the code suitable also for computations of the generalized Spitzer function in stellarators.

The code SYNCH [69] computes the generalized Spitzer function and its derivatives in the long mean free path regime in general toroidal geometry and all types of flux coordinates. Therefore it is suitable for tokamaks as well as stellarators, only the magnetic field module B and the Jacobian \sqrt{g} must be provided by the user. It is a fully relativistic code [it does not use the "weakly relativistic" expansion over $T/(m_e c^2)$] that has been originally developed for studies of passive cyclotron current drive in tokamaks [69] and has recently been upgraded to general geometry. In the context of this work SYNCH is used to compute the reference cases for the collisionless limit.

8.2 Neoclassical transport matrix

For a large aspect ratio tokamak with circular flux surfaces the coefficients γ_{ik} computed by NEO-2 are compared to the analytical results of References 38,60, 61. In particular, the dimensionless transport coefficients for the Hinton and Hazeltine model [60], γ_{ij}^{HH} , are given by $\gamma_{ij}^{\text{HH}} = K_{ij}q^2\epsilon_t^{-3/2}Z_{\text{eff}}$ for i, j = 1, 2, $\gamma_{ij}^{\text{HH}} = K_{ij}q\epsilon_t^{-1/2}/2$ for i = 1, 2 and j = 3 or i = 3 and j = 1, 2,

$$\gamma_{33}^{\text{HH}} = \frac{K_{33} \epsilon_t^{1/2} - \langle \hat{B}^2 \rangle}{2Z_{\text{eff}} \left[0.29 + 0.46 \left(1.08 + Z_{\text{eff}} \right)^{-1} \right]}$$
(8.1)

and the matrix K_{ij} is defined by Eqs. (6.125) and (6.126) of Reference 60. Here q is the safety factor and $\epsilon_t = r/R$ is the inverse aspect ratio. The results of the comparison are presented in Figs. 8.1 to 8.6 for t = 1/q = 0.362 and $\epsilon_t = 0.075$. The results of NEO-2 are computed with associated Laguerre polynomials up to fourth order and Legendre polynomials up to third order. For all coefficients the dependence on collisionality as well as Z_{eff} is well reproduced. The main differences come from the finite toroidicity. Whereas NEO-2 does not assume

smallness of the magnetic field modulation, theoretical approximations are based on the expansion over ϵ_t . It should be noted that in NEO-2 all nine transport coefficients are computed independently and Onsager symmetry of these coefficients is used for the control of the computation accuracy which improves with both, grid resolution and (mainly) number of Laguerre polynomials in modeling energy dependence (see Figs. 8.10 to 8.12). For the present computation violation of symmetries $\gamma_{13} = \gamma_{31}$ and $\gamma_{23} = \gamma_{32}$ is around 1% and violation of symmetry $\gamma_{12} = \gamma_{21}$ is around 10%.

Beside the full linearized collision operator, two different model operators are used in Figs. 8.7 to 8.9, namely, the mono-energetic collision model and mono-energetic collision model with momentum recovery. Last two models are obtained by putting in Eq. (3.26) $D_{mm'} = I_{mm'}^{(\ell)} = 0$ or only $D_{mm'} = 0$, respectively. In particular, the mono-energetic model here corresponds to the most common mono-energetic approach where transport coefficients are given by the convolution over energy of the results for the Lorentz model. It can be seen that mono-energetic model overestimates particle diffusion coefficient γ_{11} while mono-energetic model with momentum recovery underestimates this coefficient as compared to the full linearized collision model. The bootstrap coefficient γ_{31} , in turn, is underestimated by the mono-energetic model while the mono-energetic model with momentum recovery overestimates it. Finally, conductivity coefficient is well reproduced by the mono-energetic model while the mono-energetic model with momentum recovery significantly overestimates it. Differences between all three models are naturally reduced with higher $Z_{\rm eff}$. Currently NEO-2 has been and is being used for the benchmarking of various methods for the computation of mono-energetic transport coefficients and bootstrap coefficient [72, 74] as well as momentum correction techniques [73, 75].

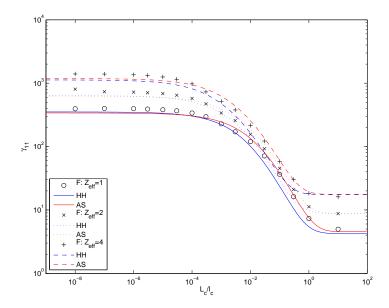


Figure 8.1: Results of NEO-2 with full linearized collision operator (F) and analytical models of Ref. 60 (HH) and Refs. 38 and 61 (AS) for the dimensionless diffusion coefficient γ_{11} at three values of the effective charge $Z_{\rm eff}$.

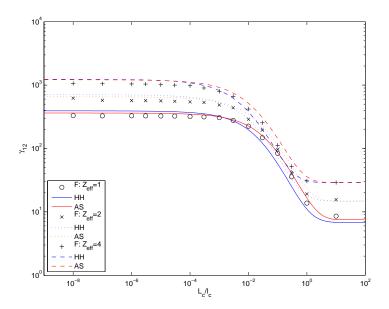


Figure 8.2: The same as in Fig.8.1 for γ_{12} .

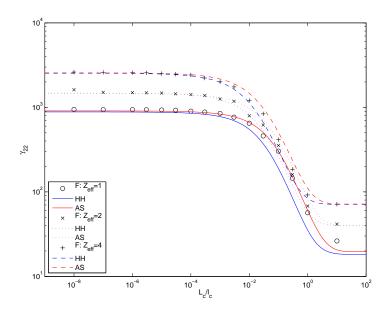


Figure 8.3: The same as in Fig.8.1 for γ_{22} .

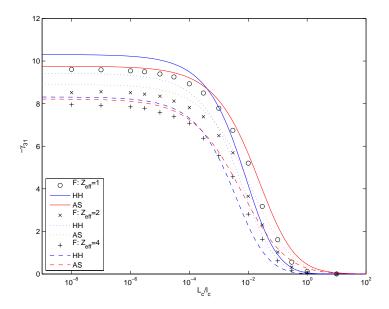


Figure 8.4: The same as in Fig.8.1 for $-\gamma_{31}$.

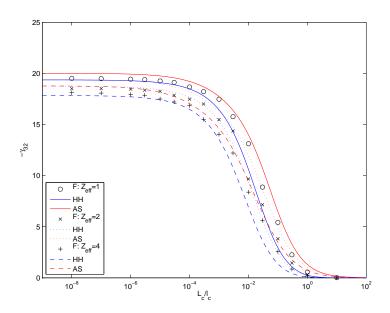


Figure 8.5: The same as in Fig.8.1 for $-\gamma_{32}$.

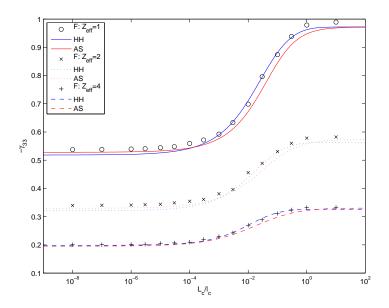


Figure 8.6: The same as in Fig.8.1 for $-\gamma_{33}$.

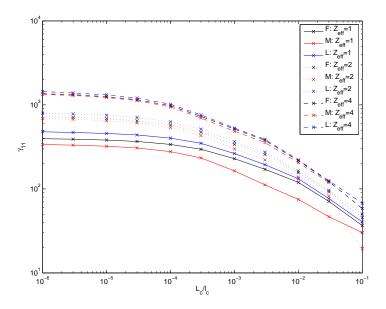


Figure 8.7: Dimensionless particle diffusion coefficient γ_{11} for the full linearized collision operator (F), mono-energetic approach (L) and mono-energetic approach with momentum recovery (M).

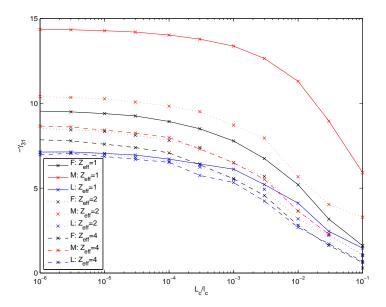


Figure 8.8: The same as in Fig. 8.7 for the bootstrap coefficient $-\gamma_{31}$

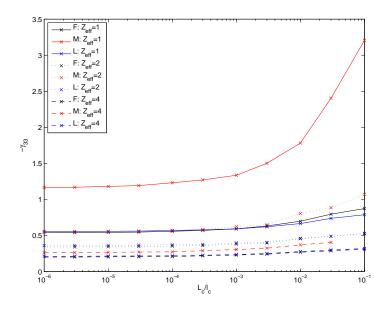


Figure 8.9: The same as in Fig. 8.7 for the conductivity coefficient $-\gamma_{33}$

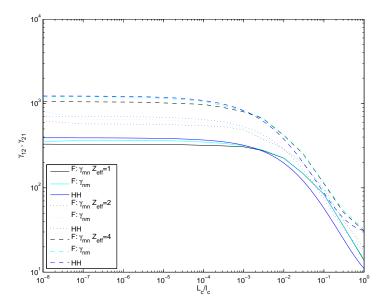


Figure 8.10: On sager symmetry for the coefficients γ_{12} and γ_{21} , respectively.

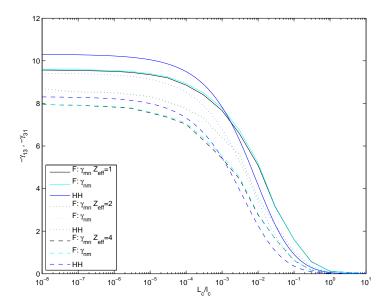


Figure 8.11: On sager symmetry for the coefficients $-\gamma_{13}$ and $-\gamma_{31}$, respectively.

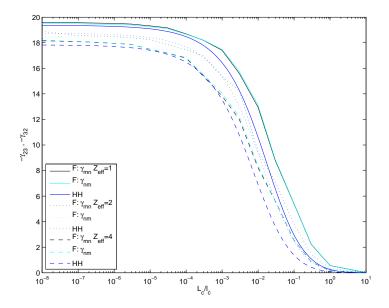


Figure 8.12: On sager symmetry for the coefficients $-\gamma_{23}$ and $-\gamma_{32}$, respectively.

8.3 Generalized Spitzer function

The resulting generalized Spitzer function has specific features which are pertinent to the finite plasma collisionality [43, 76]. They are absent in asymptotic (collisionless or highly collisional) regimes or in results drawn from interpolation between asymptotic limits. These features have the potential to improve the overall ECCD efficiency if one optimizes the microwave beam launch scenarios accordingly.

To illustrate the difference between collisional and collisionless cases, the generalized Spitzer function g and its derivatives $\partial g/\partial v_{\perp}$, $\partial g/\partial v_{\parallel}$ are presented as functions of the pitch-angle parameter $\lambda = v_{\parallel}/v$. All computations were done for a circular tokamak (see Appendix F) with major radius $R_0 = 100$ cm, minor radius r = 25 cm (A = 4), rotational transform t = 0.52, electron density $n_e = 6.65 \cdot 10^{13}$ cm⁻³, electron temperature $T_e = 1$ keV. These parameters result in collisionality $2\pi qR/(l_{\rm Sp}\epsilon_t^{3/2}) = 0.257$. For NEO-2 computations the number of Laguerre polynomials was 6.

To highlight the different aspects of the influence of collisions on g, results are presented for four different positions on the flux surface, namely B_{min} (outer side), B_{max} (inner side), top and bottom. Velocities correspond approximately to the following important transport regimes: (i) Pfirsch-Schlüter regime, $v = 0.5v_t$ (sub-thermal); (ii) plateau regime, $v = v_t$ (thermal); banana regime, $v = 2v_t$ (intermediate); and deep banana regime, $v = 3v_t$ (fast). Here, $v_t = \sqrt{2T_e/m_e}$ is the thermal velocity. Overall one sees good convergence to asymptotic limits and various collisional results which are mainly caused by a combination of the magnetic mirroring force and collisional detrapping processes. Since the adjoint generalized Spitzer function has a simple physical meaning - this is the amount of parallel current produced by a point particle source at given location in the momentum space - further on the function g is discussed in terms of particle motion in the phase space.

Minimum B point: Figure 8.13 presents the transition from sub-thermal to fast particles at the B_{min} point. One can clearly observe how collisional detrapping of particles results in current generation even from particles originally situated in the trapped region. These phenomenon gradually disappears with increasing velocity and results finally converge to the collisionless limit. Since the derivative of g with respect to the perpendicular velocity v_{\perp} is most important for ECCD, examples for $\partial g/\partial v_{\perp}$ are given in the thermal and intermediate velocity ranges, respectively, in Figure 8.14.

Maximum B **point:** Figure 8.15 shows a fundamental difference between

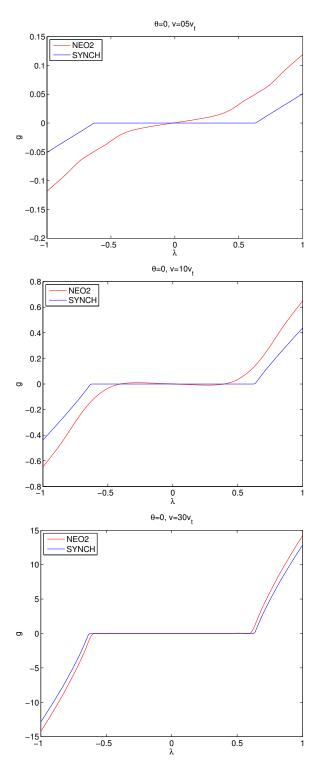


Figure 8.13: Generalized Spitzer function, g, vs. pitch parameter, λ , at the B_{min} point for $v = 0.5v_t$ (top), $v = v_t$ (middle) and $v = 3v_t$ (bottom), respectively. Results from NEO-2 (red) are compared to the collisionless limit computed by SYNCH (blue).

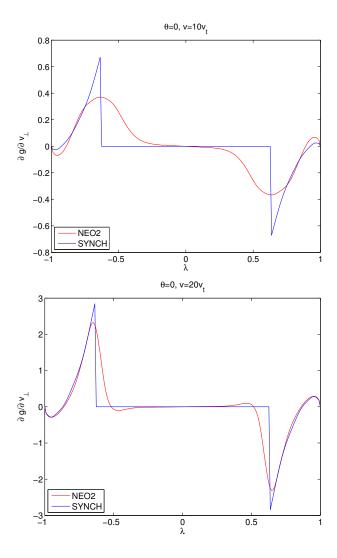


Figure 8.14: Perpendicular derivative of the generalized Spitzer function, $\partial g/\partial v_{\perp}$, vs. pitch parameter, λ , at the B_{min} point for $v=v_t$ (top) and $v=2v_t$ (bottom), respectively. Results from NEO-2 (red) are compared to the collisionless limit computed by SYNCH (blue).

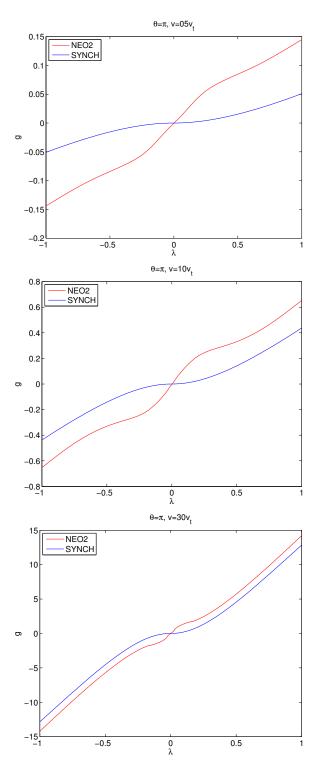


Figure 8.15: Generalized Spitzer function, g, vs. pitch parameter, λ , at the B_{max} point for $v = 0.5v_t$ (top), $v = v_t$ (middle) and $v = 3v_t$ (bottom), respectively. Results from NEO-2 (red) are compared to the collisionless limit computed by SYNCH (blue).

collisional and collisionless cases in the range of small values of the pitch parameter λ . In results from NEO-2 the functional dependence of q at small pitch values is similar to a cubic root. This is in contrast to results in the collisionless case where this dependence is closer to a cubic parabola. This rapid increase of q from NEO-2 at small pitch values is connected with acceleration of electrons by the magnetic mirror force. Very slow electrons starting from the top of the hill at B_{max} are accelerated by the magnetic mirroring force towards B_{min} . The velocity at B_{min} is almost independent on differences in small starting velocities, but is mainly determined by the change of the magnetic potential energy thus resulting in roughly the same final values. During this process of acceleration, collisions move half of those electrons deeper into the passing region so that they are not decelerated back to the starting velocity when approaching the field maximum for the next time, thus producing a finite time averaged net current before their distribution becomes a Maxwellian. Of course, this behavior is more pronounced in sub-thermal and thermal regimes but it is still present in LMFP regimes in a small vicinity of $v_{\parallel} = 0$. Further away from $v_{\parallel} = 0$, NEO-2 curves tend to a cubic parabola similar to the collisionless approach (SYNCH). Because of the importance for ECCD computations, again examples for $\partial g/\partial v_{\perp}$ are given in the thermal and intermediate velocity ranges, respectively, in Figure 8.16.

Top and bottom points: It can be seen from Figure 8.17 that antisymmetry of the generalized Spitzer function q pertinent to asymptotic regimes and to magnetic field extrema is not existing anymore since particles starting from the trapped region tend to produce the current flow in the direction of the magnetic field minimum. The sign of this current depends on the position of the source (the sign of such a current produced by a source at the top of the flux surface is opposite to the sign of the current from a source at the bottom). As pointed out in Reference 77, this feature allows to generate currents by waves with a symmetric spectrum introducing up-down asymmetry of the microwave radiation. This behavior is again the result of the magnetic mirroring force. Particles starting within the loss cone are accelerated (or decelerated) by this force so that, independent on their initial velocity, all of them finally have the same velocity sign at the magnetic field minimum point. They, however, might not reach the next maximum as trapped ones because they can be detrapped by collisions and will continue as passing ones, thus producing a net time averaged current until their distribution becomes a Maxwellian due to collisions. At higher velocities where electrons are in the banana regime, such a behavior is preserved only for trapped electrons close to the trapped passing boundary. Actually, the above feature is responsible also for the bootstrap effect [77] where the source term (gradient drive) possesses

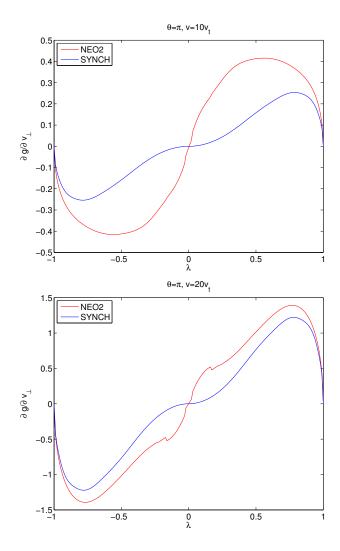


Figure 8.16: Perpendicular derivative of the generalized Spitzer function, $\partial g/\partial v_{\perp}$, vs. pitch parameter, λ , at the B_{max} point for $v=v_t$ (top) and $v=2v_t$ (bottom), respectively. Results from NEO-2 (red) are compared to the collisionless limit computed by SYNCH (blue).

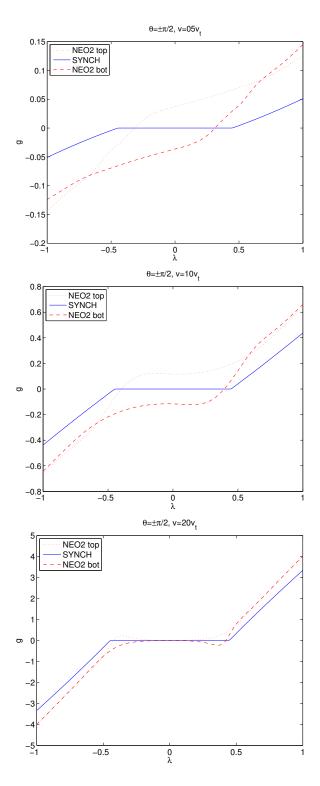


Figure 8.17: Generalized Spitzer function, g, vs. pitch parameter, λ , at the top (dashed) and bottom points (dotted) for $v=0.5v_t$ (top), $v=v_t$ (middle) and $v=2v_t$ (bottom), respectively. Results from NEO-2 (red) are compared to the collisionless limit computed by SYNCH (blue).

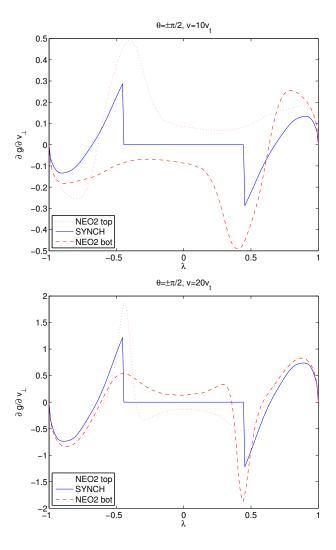


Figure 8.18: Perpendicular derivative of the generalized Spitzer function, $\partial g/\partial v_{\perp}$, vs. pitch parameter, λ , at the top (dashed) and bottom points (dotted) for $v=v_t$ (top) and $v=2v_t$ (bottom), respectively. Results from NEO-2 (red) are compared to the collisionless limit computed by SYNCH (blue).

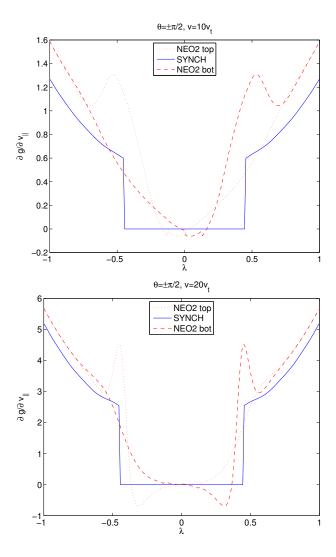


Figure 8.19: Parallel derivative of the generalized Spitzer function, $\partial g/\partial v_{\parallel}$, vs. pitch parameter, λ , at the top (dashed) and bottom points (dotted) for $v=v_t$ (top) and $v=2v_t$ (bottom), respectively. Results from NEO-2 (red) are compared to the collisionless limit computed by SYNCH (blue).

a natural up-down antisymmetry.

Formally, the loss of asymmetry of the Spitzer function in regimes with finite plasma collisionality can be seen from Eq. (4.2) where the first term on the left hand side (dynamic operator) and the second term (collision operator) have different parity properties with respect to the parallel velocity. While the collision operator conserves parity of the solution, the dynamic operator changes parity to the opposite. The sum of these operators has no definite parity which results in solutions without a definite parity. However, for either very high or very low collisionality the dynamic operator is either small or plays no role for the largest, bounce averaged part of the solution. As a result, in these limiting cases the solution has the same parity as the right hand side of Eq. (4.2), i.e. it is antisymmetric. At the same time, in a tokamak with up-down symmetry the left hand side of Eq. (4.2) preserves exactly a more general parity - parity with respect to simultaneous change of the sign of parallel velocity and of the poloidal angle. This can be seen from Figure 8.17. Such a behavior of the generalized Spitzer function g suggests a "naive" recommendation for the choice between the upper and the lower deposition points: One should choose the position of the source at the flux surface in such a way that the desired direction of the electron flow velocity (which determines the sign of parallel phase velocity of the microwaves in the case of ECCD) at the position of the source is towards the magnetic field minimum. In such a case the mirror force would serve to increase the current. However, this recommendation would be correct for a beam-like source in velocity space which does not change the sign. In the case of a ECCD source where there is a change in sign (its velocity space integral is actually zero), mainly the perpendicular derivative of q determines the effect, and, as it can be seen from Figure 8.18, there is no general trend for this derivative. For slow particles this trend is the same as for q but for fast particles the trend changes to the opposite. Since the resonant line in velocity space goes through regions with different values of the velocity module, the conclusion about the role of the mirror force in such cases can be drawn only from direct calculations of the ECCD current with a quasilinear source computed by a ray-tracing code. (In Reference 77 where the basic idea of driving the current by waves with a symmetric spectrum has been presented, a model expression for this source has been used where the velocity dependence of the quasilinear diffusion coefficient has been only due to the finite Larmor radius effect, while the

These calculations must naturally include also the parallel derivative of g (see Figure 8.19) which usually makes a smaller contribution than the perpendicular one, but its role increases if the Ohkawa effect becomes significant.

resonance condition has been omitted.)

(There, the orientation of RF-diffusion lines with respect to this boundary is of importance, and these lines cannot be truncated to $v_{\parallel}=$ const lines.) Such calculations with the help of a combination of the code NEO-2 and the ray-tracing code TRAVIS have been started recently [40].

Chapter 9

Conclusion

In this work a detailed calculation of the moments of the full linearized collision operator (collision matrix elements) has been presented. These matrix elements are employed in the drift kinetic equation solver NEO-2 for the computation of the full neoclassical transport matrix and of the generalized Spitzer function with finite collisionality in toroidal plasmas.

In order to check the accuracy the collision matrix elements have been applied to calculate the collisional Spitzer conductivity. The results show good agreement with the "exact" numerical results of Spitzer and Härm.

As an application of the matrix elements the NEO-2 code has been used to evaluate the full electron transport matrix (nine coefficients) assuming stationary ions for the standard tokamak with circular cross section. The results are in good agreement with results of analytical theory widely used in the literature. Furthermore, effects of simplifications of the linearized collision model (e.g., reduction to a Lorentz model) have been studied in order to provide a comparison with various momentum correction techniques used for the computation of transport coefficients in stellarators. Contrary to DKE solvers which use momentum correction techniques, the implementation of the full collision operator in NEO-2 has been done directly at the level of the drift kinetic equation. Thus, the NEO-2 code can calculate the complete local solution along the magnetic field line.

Moreover, the NEO-2 code has been applied to compute the generalized Spitzer function in the standard tokamak. This work has concentrated on the basic features of the generalized Spitzer function which is one of the main elements in computations of ECCD efficiency and total ECCD current in confinement regimes with finite plasma collisionality. It has been found that in regimes where the collisional detrapping time is comparable to the bounce time, particle acceleration due to the magnetic mirroring force plays an important role in the generation of plasma current from ECCD. In particular,

due to this mirroring force, there is a significant difference between upper and lower electron cyclotron resonance zones on a given flux surface in the efficiency of current drive in given toroidal direction. In tokamaks, effects of finite collisionality are important only in the plateau regime and at the beginning of the LMFP regime. For stellarators however, these effects extend further into the LMFP regime because the length of a trapped orbit becomes rather large (many toroidal turns) when approaching the trapped-passing boundary. The reflection points of such an orbit in a stellarator are close to the position of the global magnetic field maximum which is located in one point on the flux surface. In contrast, in a tokamak only one poloidal turn is needed to connect field maxima resulting in much shorter trapped orbits. The code NEO-2 turns out to be a valuable DKE-solver for ECCD problems because of the unique feature that the full linearized collision operator can be used locally. Thus the full 3D (4D) problem of local current drive efficiency can be tackled in tokamaks (stellarators). At the moment however, usage is only possible for tokamak problems due to limited speed of the code. A substantial speed-up of the code is possible with improvements of the ODEsolver and code parallelization. Such improvements are in development. Any usage for stellarators is only possible after such a speed-up. At the moment, such a first principle solver can be used to check approximate models and identify improvement possibilities for ECCD efficiency. Thorough studies including ray tracing simulations have to follow this study to provide a better insight into the topic. For this purpose, the coupling of the kinetic equation solver NEO-2 and ray-tracing code TRAVIS has been performed. Preliminary results on this topic have been presented in Reference 40.

Appendix A

Complete set of orthonormal functions

In transport theory polynomial expansions of the distribution function have been widely used for the kinetic equation. The distribution function could be expanded in any complete set of orthogonal functions, however, it turned out that associated Laguerre polynomials [29] (also called Sonine polynomials) are especially suited for transport theory problems (see, e.g., [22,78–80]). Below, two sets of orthonormal functions used in this work, namely the test functions φ_m as well as the Burnett functions, are briefly described. In the test function basis only the radial (velocity dependent) part of the perturbation of the distribution function is expanded, where in the Burnett basis the angular (pitch-angle dependent) part is expanded as well.

A.1 φ -basis

The scalar product of arbitrary functions $\alpha(v)$ and $\beta(v)$ is defined by the equation

$$(\alpha, \beta) \equiv \frac{1}{n_s v_{ts}^2} \int_0^\infty dv v^4 f_{s0}(v) \alpha(v) \beta(v), \qquad (A.1)$$

which, upon introducing the normalized speed $x = v/v_{ts}$ and substituting the Maxwellian $f_{s0}(\psi, x) = n_s/(\pi^{3/2}v_{ts}^3)e^{-x^2}$, can thus be rewritten as

$$(\alpha, \beta) = \frac{1}{\pi^{3/2}} \int_0^\infty \mathrm{d}x e^{-x^2} x^4 \alpha(x) \beta(x). \tag{A.2}$$

The countable set of test functions $\{\varphi_m(x)\}$ employed in this work to calculate the collision matrix elements is defined by

$$\varphi_m(x) \equiv \frac{\pi^{3/4}}{\sqrt{h_m}} L_m^{(3/2)}(x^2),$$
(A.3)

with radial index m = 0, 1, 2, ..., and where $L_m^{(3/2)}$ is an associated Laguerre polynomial of order 3/2. The normalization factor $h_m = \Gamma(m + 5/2)/(2m!)$ has been chosen such that the scalar product of φ_m by $\varphi_{m'}$ is orthonormal, that is

$$(\varphi_{m}, \varphi_{m'}) = \frac{1}{n_{s}v_{ts}^{2}} \int_{0}^{\infty} dv v^{4} f_{s0}(x) \varphi_{m}(x) \varphi_{m'}(x)$$

$$= \frac{1}{n_{s}v_{ts}^{2}} \int_{0}^{\infty} dv v^{4} \frac{n_{s}}{\pi^{3/2}v_{ts}^{3}} e^{-x^{2}} \frac{\pi^{3/2}}{\sqrt{h_{m}h_{m'}}} L_{m}^{(3/2)}(x^{2}) L_{m'}^{(3/2)}(x^{2})$$

$$= \frac{1}{\sqrt{h_{m}h_{m'}}} \int_{0}^{\infty} dx e^{-x^{2}} x^{4} L_{m}^{(3/2)}(x^{2}) L_{m'}^{(3/2)}(x^{2})$$

$$= \delta_{mm'}, \qquad (A.4)$$

where the orthogonality of the associated Laguerre polynomials,

$$\int_{0}^{\infty} dx e^{-x^{2}} x^{2\ell+2} L_{m}^{(\ell+1/2)}(x^{2}) L_{m'}^{(\ell+1/2)}(x^{2}) = \frac{\Gamma(\ell+m+3/2)}{2m!} \delta_{mm'}, \quad (A.5)$$

has been applied [47].

This set of test functions constitutes a complete set of functions (or basis) if an arbitrary function $G(\lambda, x)$ can be expressed in one and only one way in terms of φ_m . Hence,

$$G(\lambda, x) = \sum_{m} g_m(\lambda)\varphi_m(x). \tag{A.6}$$

From Eqs. (A.1) and (A.4) it follows that

$$(\varphi_m, G) = \frac{1}{n_s v_{ts}^2} \int_0^\infty dv v^4 f_{s0} \varphi_m G$$
$$= \frac{1}{n_s v_{ts}^2} \int_0^\infty dv v^4 f_{s0} \varphi_m \sum_{m'} g_{m'} \varphi_{m'}$$

A.1. φ -BASIS

$$= \sum_{m'} g_{m'} \frac{1}{n_s v_{ts}^2} \int_0^\infty dv v^4 f_{s0} \varphi_m \varphi_{m'}$$

$$= \sum_{m'} g_{m'} (\varphi_m, \varphi_{m'})$$

$$= \sum_{m'} g_{m'} \delta_{mm'}$$

$$= g_m(\lambda), \qquad (A.7)$$

that is, the expansion coefficient g_m of G on φ_m is therefore equal to the scalar product of G by φ_m .

The closure relation is obtained by replacing the components g_m in Eq. (A.6) by (φ_m, G) ,

$$G(x) = \sum_{m} g_{m} \varphi_{m}(x)$$

$$= \sum_{m} (\varphi_{m}, G) \varphi_{m}(x)$$

$$= \sum_{m} \frac{1}{n_{s} v_{ts}^{2}} \int_{0}^{\infty} dv' v'^{4} f_{s0}(x') \varphi_{m}(x') G(x') \varphi_{m}(x)$$

$$= \sum_{m} \frac{v_{ts}^{3}}{n_{s}} \int_{0}^{\infty} dx' x'^{4} f_{s0}(x') \varphi_{m}(x') G(x') \varphi_{m}(x)$$

$$= \int_{0}^{\infty} dx' x'^{4} G(x') \frac{v_{ts}^{3}}{n_{s}} f_{s0}(x') \sum_{m} \varphi_{m}(x') \varphi_{m}(x), \qquad (A.8)$$

where the λ dependence has been suppressed for clarity. From Eq. (A.8) the closure relation can be deduced to be

$$\frac{v_{ts}^3}{n_s} x'^4 f_{s0}(x') \sum_{m} \varphi_m(x') \varphi_m(x) \equiv \delta(x - x'), \tag{A.9}$$

where $\delta(x-x')$ is Dirac's delta function. This relation expresses the fact that the set $\{\varphi_m(x)\}$ constitutes a basis.

The collision matrix elements of the Coulomb operator C_{ab} (see Appendix B) are defined as follows,

$$(\varphi_m | \mathcal{C}_{ab} | \varphi_{m'}) \equiv \frac{1}{n_a v_{ta}^2} \int_0^\infty dv v^4 \varphi_m \mathcal{C}_{ab} [f_{a0}(v) \varphi_{m'}(x)]. \tag{A.10}$$

A.2 Burnett basis

In kinetic theory an extensively used complete set of orthonormal functions is the so-called Burnett basis (see, e.g., References 37,78,81–84). Generally, the Burnett functions, $B_n^{(\ell)}$, are products of associated Laguerre polynomials and spherical harmonics but for problems with azimuthal symmetry (which has been assumed throughout this work) the spherical harmonics can be replaced by Legendre polynomials. Thus, the Burnett functions are represented by

$$B_n^{(\ell)}(\lambda, x) = x^{\ell} L_n^{(\ell+1/2)}(x^2) P_{\ell}(\lambda) ,$$
 (A.11)

where the radial index n = 0, 1, 2, ..., and the polar index $\ell = 0, 1, 2, ...$, respectively. The Legendre polynomials P_{ℓ} form a set of orthogonal functions, that is

$$\int_{-1}^{1} d\lambda P_{\ell}(\lambda) P_{\ell'}(\lambda) = \frac{2}{2\ell+1} \delta_{\ell\ell'}.$$
 (A.12)

Upon introducing the factor

$$h_n^{(\ell)} = \frac{2}{2\ell+1} \frac{\Gamma(\ell+n+3/2)}{2\pi^{3/2}n!},\tag{A.13}$$

the normalized Burnett functions

$$b_n^{(\ell)} = \frac{B_n^{(\ell)}}{\sqrt{h_n^{(\ell)}}},\tag{A.14}$$

allows the orthonormality relation to be expressed as

$$\frac{1}{2\pi n_s} \int d^3 v \ b_n^{(\ell)} b_{n'}^{(\ell')} f_{s0} = \delta_{\ell\ell'} \delta_{nn'}. \tag{A.15}$$

Here, the scalar product is defined by

$$\langle \alpha | \beta \rangle \equiv \frac{1}{2\pi n_s} \int d^3 v f_{s0}(v) \alpha(v, \lambda) \beta(v, \lambda)$$

$$= \frac{1}{n_s} \int_{-1}^{1} d\lambda \int_{0}^{\infty} dv v^2 f_{s0}(v) \alpha(v, \lambda) \beta(v, \lambda)$$

$$= \frac{1}{\pi^{3/2}} \int_{-1}^{1} d\lambda \int_{0}^{\infty} dx e^{-x^2} x^2 \alpha(x, \lambda) \beta(x, \lambda), \qquad (A.16)$$

where the differential velocity space volume element $d^3v = v^2 dv d\lambda d\varphi$ has been used. Combining the last two equations allows the orthonormality relation to be rewritten as

$$\langle b_n^{(\ell)} | b_{n'}^{(\ell')} \rangle = \delta_{\ell \ell'} \delta_{nn'}. \tag{A.17}$$

For the case when integrations with respect to pitch-angle λ and to normalized speed x can be performed independently it might be useful to factor the scalar product $\langle \alpha | \beta \rangle$ into a pitch-angle part and a component regarding normalized speed. That is to say, providing that

$$\alpha(x,\lambda) \equiv a(\lambda)A(x)$$
 (A.18)

$$\beta(x,\lambda) \equiv b(\lambda)B(x),$$
 (A.19)

the scalar product is thus given as

$$\langle \alpha | \beta \rangle = \langle a | b \rangle_{\lambda} \langle A | B \rangle_{v}, \tag{A.20}$$

where the relations

$$\langle a|b\rangle_{\lambda} \equiv \frac{1}{2\pi} \int d\Omega ab$$

= $\int_{-1}^{1} d\lambda a(\lambda)b(\lambda),$ (A.21)

and

$$\langle A|B\rangle_v \equiv \frac{1}{n_s} \int_0^\infty dv v^2 f_{s0}(v) A(v) B(v)$$
 (A.22)

$$= \frac{1}{\pi^{3/2}} \int_{0}^{\infty} dx e^{-x^2} x^2 A(x) B(x), \tag{A.23}$$

indicate the angular and radial scalar products, respectively. The expansion of an arbitrary function $Q(\lambda, x)$ on the Burnett basis is written as

$$Q(\lambda, x) = \sum_{\ell, n} q_n^{(\ell)} b_n^{(\ell)}(\lambda, x), \tag{A.24}$$

from which it follows, by inspecting Eq. (A.16) and making use of Eq. (A.17), that

$$\langle b_n^{(\ell)}|Q\rangle = \frac{1}{2\pi n_s} \int d^3 v b_n^{(\ell)}(\lambda, x) Q(\lambda, x) f_{s0}(x)$$

$$= \frac{1}{2\pi n_s} \int d^3 v b_n^{(\ell)} f_{s0} \sum_{\ell',n'} q_{n'}^{(\ell')} b_{n'}^{(\ell')}(\lambda, x)$$

$$= \sum_{\ell',n'} q_{n'}^{(\ell')} \frac{1}{2\pi n_s} \int d^3 v b_n^{(\ell)} b_{n'}^{(\ell')} f_{s0}$$

$$= \sum_{\ell',n'} q_{n'}^{(\ell')} \langle b_n^{(\ell)} | b_{n'}^{(\ell')} \rangle$$

$$= \sum_{\ell',n'} q_{n'}^{(\ell')} \delta_{\ell\ell'} \delta_{nn'}$$

$$= q_n^{(\ell)}, \tag{A.25}$$

where the expansion coefficients $q_n^{(\ell)}$ sometimes are called Burnett moments [37]. Substituting the coefficients $q_n^{(\ell)} = \langle b_n^{(\ell)} | Q \rangle$ into the expansion of function Q,

$$Q(\lambda, x) = \sum_{\ell,n} q_n^{(\ell)} b_n^{(\ell)}(\lambda, x)$$

$$= \sum_{\ell,n} \langle b_n^{(\ell)} | Q \rangle b_n^{(\ell)}(\lambda, x)$$

$$= \sum_{\ell,n} \frac{1}{n_s} \int_{-1}^{1} d\lambda' \int_{0}^{\infty} dv' v'^2 f_{s0}(x')$$

$$\times b_n^{(\ell)}(\lambda', x') Q(\lambda', x') b_n^{(\ell)}(\lambda, x)$$

$$= \int_{-1}^{1} d\lambda' \int_{0}^{\infty} dx' x'^2 Q(\lambda', x')$$

$$\times \frac{v_{ts}^3 f_{s0}(x')}{n_s} \sum_{\ell,n} b_n^{(\ell)}(\lambda', x') b_n^{(\ell)}(\lambda, x), \quad (A.26)$$

yields the closure relation for the Burnett function basis, namely

$$\frac{v_{ts}^{3} f_{s0}(x')}{n_{s}} \sum_{\ell,n} b_{n}^{(\ell)}(\lambda', x') b_{n}^{(\ell)}(\lambda, x) = \frac{1}{x'^{2}} \delta(x - x') \delta(\lambda - \lambda'). \tag{A.27}$$

The test functions φ_m can be expressed in terms of the Burnett functions basis as

$$\varphi_m(x) = \int_{-1}^{1} d\lambda' \int_{0}^{\infty} dx' x'^2 \varphi_m(x') \frac{1}{x'^2} \delta(x - x') \delta(\lambda - \lambda')$$

$$= \int_{-1}^{1} d\lambda' \int_{0}^{\infty} dx' x'^{2} \varphi_{m}(x') \frac{v_{ts}^{3} f_{s0}(x')}{n_{s}} \sum_{\ell,n} b_{n}^{(\ell)}(\lambda', x') b_{n}^{(\ell)}(\lambda, x)$$

$$= \sum_{\ell,n} b_{n}^{(\ell)}(\lambda, x) \langle \varphi_{m} | b_{n}^{(\ell)} \rangle$$

$$= \sum_{\ell,n} \frac{b_{n}^{(\ell)}}{\sqrt{h_{n}^{(\ell)}}} \langle P_{0} | P_{\ell} \rangle_{\lambda'} \langle \varphi_{m} | p_{n}^{(\ell)} \rangle_{v'}$$

$$= 2 \sum_{r} \frac{B_{n}^{(0)}(x)}{h_{n}^{(0)}} \langle \varphi_{m} | p_{n}^{(0)} \rangle_{v'}, \qquad (A.28)$$

where Eqs. (A.21) and (A.22) along with Eq. (A.12) have been applied and the abbreviation $p_n^{(\ell)} \equiv x^\ell L_n^{(\ell+1/2)}(x^2)$ has been introduced. In Chap. 5.3.1 the normalized distribution function appeared in terms of test functions $\varphi_m(y)$ in the form $\hat{f}(y,\lambda) \equiv f_m(\lambda)\varphi_m(y)$, which can be transformed to the Burnett basis via

$$\hat{f}(y,\lambda) = \int_{-1}^{1} d\lambda' \int_{0}^{\infty} dy' y'^{2} \hat{f}(y',\lambda') \frac{1}{y'^{2}} \delta(y-y') \delta(\lambda-\lambda')
= \int_{-1}^{1} d\lambda' \int_{0}^{\infty} dy' y'^{2} \hat{f}(y',\lambda') \frac{v_{tb}^{3} f_{b0}(y')}{n_{b}} \sum_{\ell',n'} b_{n'}^{(\ell')}(y',\lambda') b_{n'}^{(\ell')}(y,\lambda)
= \sum_{\ell',n'} b_{n'}^{(\ell')}(y,\lambda) \frac{1}{n_{b}} \int_{-1}^{1} d\lambda' \int_{0}^{\infty} dv' v'^{2} \varphi_{m'}(y') f_{m'}(\lambda') f_{b0}(y') b_{n'}^{(\ell')}(y',\lambda')
= \sum_{\ell',n'} \frac{B_{n'}^{(\ell')}(y,\lambda)}{h_{n'}^{(\ell')}} \langle f_{m'} | P_{\ell'} \rangle_{\lambda'} \langle \varphi_{m'} | p_{n'}^{(\ell')} \rangle_{v'}.$$
(A.29)

Finally, the matrix elements of the Coulomb collision operator C_{ab} (see Appendix B) in terms of Burnett functions are defined as follows,

$$\langle b_n^{(\ell)} | \mathcal{C}_{ab} | b_{n'}^{(\ell')} \rangle \equiv \frac{1}{2\pi n_a} \int d^3 v b_n^{(\ell)} \mathcal{C}_{ab} \left[f_{a0}(v) b_{n'}^{(\ell')} \right]$$
$$= \frac{1}{n_a} \int_{-1}^{1} d\lambda \int_{0}^{\infty} dv v^2 b_n^{(\ell)} \mathcal{C}_{ab} \left[f_{a0}(v) b_{n'}^{(\ell')} \right]. \tag{A.30}$$

Appendix B

Coulomb collision operator

In this Appendix some useful properties of the Coulomb collision operator are reviewed. A more detailed description can be found in, e.g., References 30 and 57,58,85.

The Coulomb collision operator acting on particles of species a,

$$C_a = \sum_b C_{ab}, \tag{B.1}$$

is a sum of contributions from collisions of the scattered particles ('test particles') with the background particles ('field particles').

B.1 Landau form

The Landau form [86] of the Coulomb collision operator C_{ab} describing the effect of collisions of test particles a off field particles b can be represented as

$$C_{ab}[f_a, f_b] = \frac{\Gamma^{ab}}{m_a} \frac{\partial}{\partial \mathbf{v}} \cdot \int d^3 v' \mathbf{U}(\mathbf{u}) \cdot \left[\frac{f_b(\mathbf{v}')}{m_a} \frac{\partial f_a(\mathbf{v})}{\partial \mathbf{v}} - \frac{f_a(\mathbf{v})}{m_b} \frac{\partial f_b(\mathbf{v}')}{\partial \mathbf{v}'} \right], \quad (B.2)$$

with $\Gamma^{ab} \equiv 2\pi e_a^2 e_b^2 \ln \Lambda$, and where f_a and f_b denote the distribution functions for the scattered and background species respectively [23, 58]. Here, **U** is the so-called Landau (or scattering) tensor defined as

$$\mathbf{U}(\mathbf{u}) = \frac{1}{u} \left(\mathbf{I} - \frac{\mathbf{u}\mathbf{u}}{u^2} \right),\tag{B.3}$$

with \mathbf{I} being the unit dyadic and $\mathbf{u} = \mathbf{v} - \mathbf{v}'$. The collision operator conserves number of particles, momentum and energy [22, 23, 58], i.e.,

$$\int d^3 v \mathcal{C}_{ab} = 0 \tag{B.4}$$

$$\int d^3 v m_a \mathbf{v} \mathcal{C}_{ab} = -\int d^3 v m_b \mathbf{v} \mathcal{C}_{ba}$$
 (B.5)

$$\int d^3v \frac{m_a v^2}{2} \mathcal{C}_{ab} = -\int d^3v \frac{m_b v^2}{2} \mathcal{C}_{ba}.$$
 (B.6)

From Eq. (B.2) one can see that the operator has the form of a divergence of a vector representing the flux in velocity space due to collisions between particles [58, 87, 88],

$$C_{ab} = -\nabla \cdot \mathbf{j}^{ab},\tag{B.7}$$

with $\nabla \equiv \partial/\partial \mathbf{v}$ being the divergence in velocity space and

$$\mathbf{j}^{ab} = \frac{\Gamma^{ab}}{m_a} \int d^3 v' \mathbf{U}(\mathbf{u}) \cdot \left[\frac{f_a(\mathbf{v})}{m_b} \frac{\partial f_b(\mathbf{v'})}{\partial \mathbf{v'}} - \frac{f_b(\mathbf{v'})}{m_a} \frac{\partial f_a(\mathbf{v})}{\partial \mathbf{v}} \right]. \tag{B.8}$$

The collision term is often expressed in a standard Fokker-Planck form

$$C_{ab} = \frac{\partial}{\partial \mathbf{v}} \cdot \left[\mathbf{D} \cdot \frac{\partial f}{\partial \mathbf{v}} - \frac{1}{m} \mathbf{F} f \right], \tag{B.9}$$

where **D** is the velocity space diffusion tensor and **F** is the force of dynamical friction [23]. By comparing Eqs. (B.7) and (B.8) with Eq. (B.9) one can identify the Fokker-Planck coefficients

$$\mathbf{D}^{ab}(f_b) \equiv \frac{\Gamma^{ab}}{m_a^2} \int d^3 v' \mathbf{U}(\mathbf{u}) f_b(\mathbf{v'})$$
 (B.10)

and

$$\mathbf{F}^{ab}(f_b) \equiv \frac{\Gamma^{ab}}{m_b} \int d^3 v' \mathbf{U}(\mathbf{u}) \cdot \frac{\partial f_b(\mathbf{v'})}{\partial \mathbf{v'}}, \tag{B.11}$$

respectively. The particle flux density in velocity space can thus be rewritten in the form

$$\mathbf{j}^{ab} = \frac{1}{m_a} \mathbf{F}^{ab} f_a - \mathbf{D}^{ab} \cdot \nabla f_a. \tag{B.12}$$

B.2 RMJ form

The Landau form of the collision term is convenient only for analytical calculations. However, for numerical evaluation this operator is hardly manageable [because of the Landau tensor, the derivatives with respect to velocity and integration over velocity of the background particles, see Eq. (B.8)]. A tractable form is due to Rosenbluth, MacDonald and Judd (see Reference 89) who recognized analogies with electrostatics and defined two scalar quantities

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('Rosenbluth potentials') expressing the contributions of the background species b to the diffusion tensor and friction force [23]. These potentials are defined as

$$h_a(\mathbf{v}) \equiv \sum_b \left(1 + \frac{m_a}{m_b}\right) \int d^3 v' \frac{f_b(\mathbf{v}')}{u}$$
 (B.13)

$$g(\mathbf{v}) \equiv \sum_{b} \int d^{3}v' u f_{b}(\mathbf{v}'),$$
 (B.14)

and may be calculated by decomposing the background distribution function f_b in terms of, e.g., spherical harmonics [57] (see also Appendix C).

In the present work the more convenient notation of Trubnikov is used [58]. The so-called 'Trubnikov potentials' are defined as

$$\varphi_b(\mathbf{v}) \equiv -\frac{1}{4\pi} \int d^3 v' \frac{f_b(\mathbf{v}')}{u}$$
 (B.15)

$$\psi_b(\mathbf{v}) \equiv -\frac{1}{8\pi} \int d^3 v' u f_b(\mathbf{v}'), \tag{B.16}$$

and they are related to the Rosenbluth potentials by means of the equations

$$h_a(\mathbf{v}) = -4\pi \sum_b \left(1 + \frac{m_a}{m_b}\right) \varphi_b(\mathbf{v})$$
 (B.17)

$$g(\mathbf{v}) = -8\pi \sum_{b} \psi_b(\mathbf{v}). \tag{B.18}$$

By virtue of the following properties of the Landau tensor,

$$\mathbf{U} = \nabla \nabla u \tag{B.19}$$

$$\nabla \cdot \mathbf{U} = \nabla \frac{2}{u}, \tag{B.20}$$

the diffusion tensor as well as the force of dynamical friction can be expressed as

$$\mathbf{D}^{ab} = -L^{ab} \nabla \nabla \psi_b \tag{B.21}$$

and

$$\mathbf{F}^{ab} = -\frac{m_a^2}{m_b} L^{ab} \nabla \varphi_b, \tag{B.22}$$

respectively. Here, L^{ab} is defined by

$$L^{ab} \equiv \frac{8\pi}{m_a^2} \Gamma^{ab} = \left(\frac{4\pi e_a e_b}{m_a}\right)^2 \ln \Lambda. \tag{B.23}$$

To obtain Eq. (B.22), Eq. (B.11) has been integrated by parts and $(\partial/\partial \mathbf{v}') \cdot \mathbf{U} = -(\partial/\partial \mathbf{v}) \cdot \mathbf{U}$ has been used. Calculating the divergence of the diffusion tensor and with the help of the vector identity $\nabla^2 \mathbf{a} = \nabla(\nabla \cdot \mathbf{a}) - \nabla \times \nabla \times \mathbf{a}$ one can show that \mathbf{F}^{ab} and \mathbf{D}^{ab} are related to each other,

$$\mathbf{F}^{ab} = \frac{m_a^2}{m_b} \nabla \cdot \mathbf{D}^{ab}. \tag{B.24}$$

After substituting Eqs. (B.21) and (B.22) into Eq. (B.9) the collision operator in terms of Trubnikov potentials reads

$$C_{ab}[f_a, f_b] = L^{ab} \nabla \cdot \left[\frac{m_a}{m_b} \left(\nabla \varphi_b \right) f_a - \left(\nabla \nabla \psi_b \right) \cdot \nabla f_a \right]. \tag{B.25}$$

Hence, by employing these potentials the integro-differential operator in Eq. (B.2) is converted into a differential operator when the Trubnikov potentials are explicitly provided [90].

It follows from the identities

$$\nabla^2 u = \frac{2}{u} \tag{B.26}$$

$$\nabla^2 \frac{1}{u} = -4\pi \delta(\mathbf{u}), \tag{B.27}$$

that the Trubnikov potentials satisfy the following differential equations [58]

$$\nabla^2 \psi_b = \varphi_b \tag{B.28}$$

$$\nabla^2 \varphi_b = f_b, \tag{B.29}$$

which reflects the similarity between these functionals to the electrostatic potential (Poisson's equation).

B.3 Linearized operator

When a plasma is not far from thermodynamic equilibrium the distribution function of a particles species s is nearly Maxwellian and may be expanded as

$$f_s(\mathbf{v}) = f_{s0}(v) + f_{s1}(\mathbf{v}) ,$$
 (B.30)

where the perturbation f_{s1} is assumed to be relatively small, that is $f_{s1}/f_{s0} \sim \epsilon \ll 1$. Hence the collision operator can be expressed as

$$C_{ab}[f_a, f_b] = C_{ab}[f_{a0}, f_{b0}] + C_{ab}^l[f_{a1}, f_{b1}] + C_{ab}[f_{a1}, f_{b1}],$$
(B.31)

with C_{ab}^l representing the linearized operator

$$C_{ab}^{l}[f_{a1}, f_{b1}] \equiv C_{ab}[f_{a1}, f_{b0}] + C_{ab}[f_{a0}, f_{b1}]. \tag{B.32}$$

The first term on the RHS of Eq. (B.31) vanishes for the case when both distribution functions are Maxwellians at the same temperature $T_a = T_b = T$, whereas the third term, $C_{ab}[f_{a1}, f_{b1}]$, indicates the nonlinear part of the collision operator which is of order ϵ^2 and thus will be neglected.

The first term on the RHS of Eq. (B.32) is a differential operator acting upon f_{a1} ('test particle part') while the second term is an integral operator acting upon f_{b1} ('field particle part'). The linearized collision operator obeys the same conservation laws as the full operator (see, e.g., Reference 85).

B.4 Collision operator in curvilinear coordinates

In the following chapter the expression for the Coulomb collision operator will be represented in covariant form valid for arbitrary curvilinear velocity-space coordinates (ξ^1, ξ^2, ξ^3) (see, e.g., References 23 and 89).

From Eq. (B.7) and after recalling the expression for the divergence of a vector field in arbitrary curvilinear coordinates [91] the covariant representation of the Coulomb collision operator can be written as

$$C_{ab} = -\frac{1}{\sqrt{g}} \frac{\partial}{\partial \xi^i} \left(\sqrt{g} g^{ik} j_k^{ab} \right), \tag{B.33}$$

with the following components for collision flux [see Eq. (B.12)],

$$j_k^{ab} = \frac{f_a}{m_a} F_k^{ab} - \left(\mathbf{D}^{ab} \cdot \nabla f_a \right)_k . \tag{B.34}$$

By means of Eqs. (B.21) and (B.22) the covariant components on the RHS of Eq. (B.34) are

$$F_k^{ab} = -\frac{m_a^2}{m_b} L^{ab} \frac{\partial \varphi_b}{\partial \xi^k}$$
 (B.35)

$$\left(\mathbf{D}^{ab} \cdot \nabla f_a\right)_k = \mathsf{D}_{kl}^{ab} g^{lm} \frac{\partial f_a}{\partial \varepsilon^m}, \tag{B.36}$$

with

$$\mathsf{D}_{kl}^{ab} = \mathsf{D}_{lk}^{ab} = -L^{ab} \left(\frac{\partial^2 \psi_b}{\partial \xi^k \partial \xi^l} - \Gamma_{kl}^n \frac{\partial \psi_b}{\partial \xi^n} \right). \tag{B.37}$$

Here, Γ is the Christoffel symbol of the second kind [91] defined by

$$\Gamma_{ik}^{j} \equiv \frac{1}{2} g^{jn} \left[\frac{\partial g_{ni}}{\partial \xi^{k}} + \frac{\partial g_{nk}}{\partial \xi^{i}} - \frac{\partial g_{ik}}{\partial \xi^{n}} \right]. \tag{B.38}$$

The Christoffel symbols are symmetric in the lower two indices, $\Gamma_{ik}^j = \Gamma_{ki}^j$. As usual, a sum over repeated indices is implied unless otherwise stated.

B.4.1 Spherical velocity-space coordinates

As an application of the results provided in the previous section the linearized collision operator will be derived in spherical velocity-space coordinates. The metric tensor g_{ij} of this orthogonal coordinate system $(\xi^1, \xi^2, \xi^3) = (v, \lambda, \varphi)$ is diagonal, with

$$g_{11} = 1,$$
 $g_{22} = \frac{v^2}{(1 - \lambda^2)},$ $g_{33} = v^2(1 - \lambda^2),$ (B.39)

where $\lambda = v_{\parallel}/v = \cos\theta$ is the cosine of the pitch-angle and φ is the gyrophase angle, respectively, and with

$$g^{ik} = \frac{1}{g_{ik}}. (B.40)$$

From Eq. (B.39) one immediately obtains the Jacobian of this coordinate system, that is to say $\sqrt{g} = v^2$. According to Eqs. (B.38)-(B.40) the only nonvanishing Christoffel symbols are

$$\Gamma_{22}^1 = -\frac{v}{(1-\lambda^2)}, \qquad \Gamma_{33}^1 = -v(1-\lambda^2),$$
(B.41)

$$\Gamma_{12}^2 = \Gamma_{21}^2 = \frac{1}{v}, \qquad \Gamma_{22}^2 = \frac{\lambda}{(1 - \lambda^2)}, \qquad \Gamma_{33}^2 = \lambda(1 - \lambda^2), \tag{B.42}$$

$$\Gamma_{13}^3 = \Gamma_{31}^3 = \frac{1}{v}, \qquad \Gamma_{23}^3 = \Gamma_{32}^3 = -\frac{\lambda}{(1-\lambda^2)}.$$
(B.43)

B.4.2 Test particle part

The test particle operator (differential part), $C_{ab}[f_{a1}, f_{b0}]$, describing the collisions of an arbitrary species a with a Maxwellian background species b is now calculated in spherical velocity-space coordinates. The distribution function for the background particles is given by the Maxwellian

$$f_b(\mathbf{v}) \equiv f_{b0}(v) = \frac{n_b}{\pi^{3/2} v_{tb}^3} e^{-(v/v_{tb})^2}.$$
 (B.44)

As a consequence of Eq. (B.44) the Trubnikov potentials only depend on the magnitude of \mathbf{v} , that is

$$\varphi_b(\mathbf{v}) = \varphi_b(v) \equiv \varphi_{b0}$$
 (B.45)

$$\psi_b(\mathbf{v}) = \psi_b(v) \equiv \psi_{b0}. \tag{B.46}$$

From Eqs. (B.34) one obtains the collisional particle flux

$$j_k^{ab} = \frac{f_{a1}}{m_a} F_k^{ab} - \left(\mathbf{D}^{ab} \cdot \nabla f_{a1} \right)_k , \qquad (B.47)$$

wherein the covariant components of the diffusion tensor (in terms of ψ_{b0}) in (v, λ, φ) coordinates [see Eq. (B.37)] can be written as

$$\mathsf{D}_{kl}^{ab} = \mathsf{D}_{lk}^{ab} = -L^{ab} \left(\frac{\partial^2 \psi_{b0}}{\partial \xi^k \partial \xi^l} - \Gamma_{kl}^n \frac{\partial \psi_{b0}}{\partial \xi^n} \right). \tag{B.48}$$

Applying the results of Section B.4.1 the particular components become

$$\mathsf{D}_{vv}^{ab} = -L^{ab} \left(\frac{\partial^2 \psi_{b0}}{\partial v^2} - \Gamma_{11}^n \frac{\partial \psi_{b0}}{\partial \xi^n} \right) \tag{B.49}$$

$$= -L^{ab} \frac{\partial^2 \psi_{b0}}{\partial v^2} = \frac{v^2}{2} \nu_{\parallel}^{ab}(v), \qquad (B.50)$$

$$\mathsf{D}_{v\lambda}^{ab} = \mathsf{D}_{\lambda v}^{ab} = -L^{ab} \left(\frac{\partial^2 \psi_{b0}}{\partial v \partial \lambda} - \Gamma_{12}^n \frac{\partial \psi_{b0}}{\partial \xi^n} \right) = 0, \tag{B.51}$$

$$\mathsf{D}_{v\varphi}^{ab} = \mathsf{D}_{\varphi v}^{ab} = -L^{ab} \left(\frac{\partial^2 \psi_{b0}}{\partial v \partial \varphi} - \Gamma_{13}^n \frac{\partial \psi_{b0}}{\partial \xi^n} \right) = 0, \tag{B.52}$$

$$\mathsf{D}_{\lambda\lambda}^{ab} = -L^{ab} \left(\frac{\partial^2 \psi_{b0}}{\partial \lambda^2} - \Gamma_{22}^n \frac{\partial \psi_{b0}}{\partial \xi^n} \right) \tag{B.53}$$

$$= -L^{ab} \left(-\Gamma_{22}^1 \frac{\partial \psi_{b0}}{\partial v} \right) \tag{B.54}$$

$$= -L^{ab} \frac{v}{(1-\lambda^2)} \frac{\partial \psi_{b0}}{\partial v} = \frac{v^4}{2(1-\lambda^2)} \nu_D^{ab}(v),$$
 (B.55)

$$\mathsf{D}_{\lambda\varphi}^{ab} = \mathsf{D}_{\varphi\lambda}^{ab} = -L^{ab} \left(\frac{\partial^2 \psi_{b0}}{\partial \lambda \partial \varphi} - \Gamma_{23}^n \frac{\partial \psi_{b0}}{\partial \xi^n} \right) = 0, \tag{B.56}$$

as well as

$$\mathsf{D}_{\varphi\varphi}^{ab} = -L^{ab} \left(\frac{\partial^2 \psi_{b0}}{\partial \varphi^2} - \Gamma_{33}^n \frac{\partial \psi_{b0}}{\partial \xi^n} \right) \tag{B.57}$$

$$= -L^{ab} \left(-\Gamma_{33}^1 \frac{\partial \psi_{b0}}{\partial v} \right) \tag{B.58}$$

$$= -L^{ab}v(1-\lambda^2)\frac{\partial\psi_{b0}}{\partial v} = \frac{v^4}{2}(1-\lambda^2)\nu_D^{ab}(v), \qquad (B.59)$$

where the parallel velocity diffusion frequency

$$\nu_{\parallel}^{ab}(v) \equiv -\frac{2L^{ab}}{v^2} \frac{\partial^2 \psi_{b0}}{\partial v^2},\tag{B.60}$$

and the deflection frequency

$$\nu_D^{ab}(v) \equiv -\frac{2L^{ab}}{v^3} \frac{\partial \psi_{b0}}{\partial v} \tag{B.61}$$

have been introduced [22], respectively. Using the expression for the physical components of a second-order tensor,

$$\hat{\mathsf{D}}_{ik} = \sqrt{g^{ii}g^{kk}}\mathsf{D}_{ik}\,,\quad\text{no summation}$$
 (B.62)

as well as Eqs. (B.39)-(B.40) the diffusion tensor for collisions of arbitrary particles with a Maxwellian background is given by

$$\hat{\mathsf{D}}_{ik}^{ab} = \frac{v^2}{2} \begin{pmatrix} \nu_{\parallel}^{ab} & 0 & 0\\ 0 & \nu_{D}^{ab} & 0\\ 0 & 0 & \nu_{D}^{ab} \end{pmatrix}. \tag{B.63}$$

The covariant components of the force of dynamical friction (in terms of φ_{b0}),

$$F_k^{ab} = -\frac{m_a^2}{m_b} L^{ab} \frac{\partial \varphi_{b0}}{\partial \xi^k},\tag{B.64}$$

in spherical velocity-space coordinates are

$$F_v^{ab} = -\frac{m_a^2}{m_b} L^{ab} \frac{\partial \varphi_{b0}}{\partial v}$$
 (B.65)

$$= -\frac{m_a^2}{(m_a + m_b)} v \nu_s^{ab}(v)$$
 (B.66)

$$F_{\lambda}^{ab} = -\frac{m_a^2}{m_b} L^{ab} \frac{\partial \varphi_{b0}}{\partial \lambda} = 0$$
 (B.67)

$$F_{\varphi}^{ab} = -\frac{m_a^2}{m_b} L^{ab} \frac{\partial \varphi_{b0}}{\partial \varphi} = 0 , \qquad (B.68)$$

with

$$\nu_s^{ab}(v) \equiv L^{ab} \left(1 + \frac{m_a}{m_b} \right) \frac{1}{v} \frac{\partial \varphi_{b0}}{\partial v}$$
 (B.69)

being the slowing down frequency [22]. The physical components can be calculated using $\hat{F}_k = \sqrt{g^{kk}} F_k$ (no summation) from which it follows that

$$\hat{F}_k = -\frac{m_a^2}{(m_a + m_b)} v\left(\nu_s^{ab}, 0, 0\right). \tag{B.70}$$

The Trubnikov potentials for a Maxwellian distribution function will be evaluated in Appendix C.3. Here only the results are given,

$$\frac{\partial \varphi_{b0}}{\partial v} = \frac{n_b}{2\pi v_{tb}^2} G(v/v_{tb}) \tag{B.71}$$

$$\frac{\partial \psi_{b0}}{\partial v} = \frac{n_b}{8\pi} [G(v/v_{tb}) - \phi(v/v_{tb})] \tag{B.72}$$

$$\frac{\partial^2 \psi_{b0}}{\partial v^2} = -\frac{n_b}{4\pi} \frac{G(v/v_{tb})}{v},\tag{B.73}$$

where ϕ denotes the error function and G is the Chandrasekhar function (for details see Appendix C.3), which allows one to express the three collision frequencies, Eqs. (B.60), (B.61) and (B.69), in conventional form

$$\nu_{\parallel}^{ab}(v) = 2\hat{\nu}_{ab} \frac{G(v/v_{tb})}{(v/v_{ta})^3}$$
(B.74)

$$\nu_D^{ab}(v) = \hat{\nu}_{ab} \frac{\phi(v/v_{tb}) - G(v/v_{tb})}{(v/v_{ta})^3}$$
(B.75)

$$\nu_s^{ab}(v) = \hat{\nu}_{ab} \frac{2T_a}{T_b} \left(1 + \frac{m_b}{m_a} \right) \frac{G(v/v_{tb})}{(v/v_{ta})},$$
 (B.76)

with

$$\hat{\nu}_{ab} = \frac{4\pi n_b e_a^2 e_b^2}{m_a^2 v_{ta}^3} \ln \Lambda \tag{B.77}$$

being the basic collision frequency [22].

By means of Eq. (B.36) the covariant components of the dot product between the diffusion tensor \mathbf{D}^{ab} and the gradient of the distribution function f_{a1} are given as

where in the last equation an orthogonal coordinate system has been assumed. Therefore, from this equation and with the results obtained above it follows that

$$\left(\mathbf{D}^{ab} \cdot \nabla f_{a1}\right)_{v} = \mathsf{D}_{vv} \frac{\partial f_{a1}}{\partial v} \tag{B.79}$$

$$\left(\mathbf{D}^{ab} \cdot \nabla f_{a1}\right)_{\lambda} = \mathsf{D}_{\lambda\lambda} \frac{(1-\lambda^2)}{v^2} \frac{\partial f_{a1}}{\partial \lambda} \tag{B.80}$$

$$\left(\mathbf{D}^{ab} \cdot \nabla f_{a1}\right)_{\varphi} = \frac{\mathsf{D}_{\varphi\varphi}}{v^{2}(1-\lambda^{2})} \frac{\partial f_{a1}}{\partial \varphi}. \tag{B.81}$$

Recalling Eq. (B.47),

$$j_k^{ab} = \frac{f_{a1}}{m_a} F_k^{ab} - \left(\mathbf{D}^{ab} \cdot \nabla f_{a1} \right)_k,$$
 (B.82)

and upon inserting Eqs. (B.66) and (B.79) the covariant v-component of collision flux \mathbf{j}^{ab} can be written down as

$$j_{v}^{ab} = \frac{f_{a1}}{m_{a}} F_{v}^{ab} - \left(\mathbf{D}^{ab} \cdot \nabla f_{a1}\right)_{v}$$

$$= -\frac{f_{a1}}{m_{a}} \frac{m_{a}^{2}}{(m_{a} + m_{b})} v \nu_{s}^{ab} - D_{vv} \frac{\partial f_{a1}}{\partial v}$$

$$= -\frac{m_{a}}{(m_{a} + m_{b})} v \nu_{s}^{ab} f_{a1} - \frac{v^{2}}{2} \nu_{\parallel}^{ab} \frac{\partial f_{a1}}{\partial v}. \tag{B.83}$$

Similarly, the covariant λ - and φ -components can now be evaluated yielding

$$j_{\lambda}^{ab} = \frac{f_{a1}}{m_a} F_{\lambda}^{ab} - \left(\mathbf{D}^{ab} \cdot \nabla f_{a1}\right)_{\lambda}$$

$$= -D_{\lambda\lambda} \frac{(1-\lambda^2)}{v^2} \frac{\partial f_{a1}}{\partial \lambda}$$

$$= -\frac{v^2}{2} \nu_D^{ab} \frac{\partial f_{a1}}{\partial \lambda}, \tag{B.84}$$

and

$$j_{\varphi}^{ab} = \frac{f_{a1}}{m_a} F_{\varphi}^{ab} - \left(\mathbf{D}^{ab} \cdot \nabla f_{a1}\right)_{\varphi}$$

$$= -\frac{D_{\varphi\varphi}}{v^2 (1 - \lambda^2)} \frac{\partial f_{a1}}{\partial \varphi}$$

$$= -\frac{v^2}{2} \nu_D^{ab} \frac{\partial f_{a1}}{\partial \varphi}, \tag{B.85}$$

respectively. Substituting the expressions for j_k^{ab} in spherical velocity-space coordinates into Eq. (B.33) one finds

$$C_{ab}[f_{a1}, f_{b0}] = -\frac{1}{\sqrt{g}} \frac{\partial}{\partial \xi^i} \left(\sqrt{g} g^{ik} j_k^{ab} \right)$$

$$= -\frac{1}{\sqrt{g}} \left[\frac{\partial}{\partial \xi^{1}} \left(\sqrt{g} g^{1k} j_{k}^{ab} \right) + \frac{\partial}{\partial \xi^{2}} \left(\sqrt{g} g^{2k} j_{k}^{ab} \right) + \frac{\partial}{\partial \xi^{3}} \left(\sqrt{g} g^{3k} j_{k}^{ab} \right) \right]$$

$$= -\frac{1}{\sqrt{g}} \left[\frac{\partial}{\partial \xi^{1}} \left(\sqrt{g} g^{11} j_{1}^{ab} \right) + \frac{\partial}{\partial \xi^{2}} \left(\sqrt{g} g^{22} j_{2}^{ab} \right) + \frac{\partial}{\partial \xi^{3}} \left(\sqrt{g} g^{33} j_{3}^{ab} \right) \right]$$

$$= -\frac{1}{v^{2}} \left[\frac{\partial}{\partial v} \left(v^{2} j_{v}^{ab} \right) + \frac{\partial}{\partial \lambda} \left((1 - \lambda^{2}) j_{\lambda}^{ab} \right) + \frac{\partial}{\partial \varphi} \left(\frac{j_{\varphi}^{ab}}{1 - \lambda^{2}} \right) \right]$$

$$= \frac{1}{v^{2}} \frac{\partial}{\partial v} \left[v^{3} \left(\frac{m_{a}}{m_{a} + m_{b}} \nu_{s}^{ab} f_{a1} + \frac{v}{2} \nu_{\parallel}^{ab} \frac{\partial f_{a1}}{\partial v} \right) \right]$$

$$+ \frac{\nu_{D}^{ab}}{2} \frac{\partial}{\partial \lambda} \left((1 - \lambda^{2}) \frac{\partial f_{a1}}{\partial \lambda} \right) + \frac{\nu_{D}^{ab}}{2(1 - \lambda^{2})} \frac{\partial^{2} f_{a1}}{\partial \varphi^{2}}. \tag{B.86}$$

Upon introducing the pitch-angle scattering (or Lorentz) operator

$$\mathcal{L} \equiv \frac{1}{2} \left[\frac{\partial}{\partial \lambda} (1 - \lambda^2) \frac{\partial}{\partial \lambda} + \frac{1}{(1 - \lambda^2)} \frac{\partial^2}{\partial \varphi^2} \right], \tag{B.87}$$

the resulting expression for the test particle part of the linearized Coulomb collision operator finally reads

$$C_{ab}[f_{a1}, f_{b0}] = \nu_D^{ab} \mathcal{L}[f_{a1}] + \frac{1}{v^2} \frac{\partial}{\partial v} \left[v^3 \left(\frac{m_a}{m_a + m_b} \nu_s^{ab} f_{a1} + \frac{v}{2} \nu_{\parallel}^{ab} \frac{\partial f_{a1}}{\partial v} \right) \right].$$
 (B.88)

B.4.3 Field particle part

The field particle operator (integral part) $C_{ab}[f_{a0}, f_{b1}]$ includes the fact that the test particles also change the state of the background species (field particles) and thus involves the Trubnikov potentials of the non-Maxwellian part of the distribution function [22, 37]. Here, the test particle species a is described by a Maxwellian distribution

$$f_a(\mathbf{v}) \equiv f_{a0}(v) = \frac{n_a}{\pi^{3/2} v_{ta}^3} e^{-(v/v_{ta})^2},$$
 (B.89)

which, according to Eq. (B.36), leads to the following expressions

$$(\mathbf{D} \cdot \nabla f_{a0})_{k} = \mathsf{D}_{kl} g^{lm} \frac{\partial f_{a0}}{\partial \xi^{m}}$$

$$= \mathsf{D}_{kl} \left(g^{l1} \frac{\partial f_{a0}}{\partial \xi^{1}} + g^{l2} \frac{\partial f_{a0}}{\partial \xi^{2}} + g^{l3} \frac{\partial f_{a0}}{\partial \xi^{3}} \right)$$

$$= D_{k1}g^{11}\frac{\partial f_{a0}}{\partial \xi^{1}}$$

$$= D_{kv}\frac{\partial f_{a0}}{\partial v} = -D_{kv}\frac{2v}{v_{ta}^{2}}f_{a0}, \qquad (B.90)$$

wherein the covariant components of the diffusion tensor in terms of ψ_{b1} [see Eq. (B.37)] are given as

$$\mathsf{D}_{kv}^{ab} = -L^{ab} \left(\frac{\partial^2 \psi_{b1}}{\partial \xi^k \partial v} - \Gamma_{k1}^n \frac{\partial \psi_{b1}}{\partial \xi^n} \right). \tag{B.91}$$

Thus, in spherical velocity-space coordinates the particular covariant components of Eq. (B.91) become

$$D_{vv}^{ab} = -L^{ab} \left(\frac{\partial^{2} \psi_{b1}}{\partial v^{2}} - \Gamma_{11}^{n} \frac{\partial \psi_{b1}}{\partial \xi^{n}} \right)$$

$$= -L^{ab} \frac{\partial^{2} \psi_{b1}}{\partial v^{2}}$$

$$D_{\lambda v}^{ab} = -L^{ab} \left(\frac{\partial^{2} \psi_{b1}}{\partial \lambda \partial v} - \Gamma_{21}^{n} \frac{\partial \psi_{b1}}{\partial \xi^{n}} \right)$$

$$= -L^{ab} \left(\frac{\partial^{2} \psi_{b1}}{\partial \lambda \partial v} - \frac{1}{v} \frac{\partial \psi_{b1}}{\partial \lambda} \right)$$

$$D_{\varphi v}^{ab} = -L^{ab} \left(\frac{\partial^{2} \psi_{b1}}{\partial \varphi \partial v} - \Gamma_{31}^{n} \frac{\partial \psi_{b1}}{\partial \xi^{n}} \right)$$

$$= -L^{ab} \left(\frac{\partial^{2} \psi_{b1}}{\partial \varphi \partial v} - \frac{1}{v} \frac{\partial \psi_{b1}}{\partial \varphi} \right) ,$$
(B.94)

where again the results of Chapter B.4.1 have been applied. Using Eq. (B.90) as well as Eqs. (B.92)-(B.94) one obtains

$$(\mathbf{D} \cdot \nabla f_{a0})_v = L^{ab} \frac{\partial^2 \psi_{b1}}{\partial v^2} \frac{2v}{v_{ta}^2} f_{a0}$$
(B.95)

$$(\mathbf{D} \cdot \nabla f_{a0})_{\lambda} = L^{ab} \left(\frac{\partial^2 \psi_{b1}}{\partial \lambda \partial v} - \frac{1}{v} \frac{\partial \psi_{b1}}{\partial \lambda} \right) \frac{2v}{v_{ta}^2} f_{a0}$$
 (B.96)

$$(\mathbf{D} \cdot \nabla f_{a0})_{\varphi} = L^{ab} \left(\frac{\partial^2 \psi_{b1}}{\partial \varphi \partial v} - \frac{1}{v} \frac{\partial \psi_{b1}}{\partial \varphi} \right) \frac{2v}{v_{ta}^2} f_{a0}.$$
 (B.97)

The covariant components of the force of dynamical friction in terms of the non-Maxwellian part of the first Trubnikov potential φ_b is evaluated from Eq. (B.35),

$$F_k^{ab} = -\frac{m_a^2}{m_b} L^{ab} \frac{\partial \varphi_{b1}}{\partial \xi^k}, \tag{B.98}$$

from which it follows that

$$F_v^{ab} = -\frac{m_a^2}{m_b} L^{ab} \frac{\partial \varphi_{b1}}{\partial v}$$

$$F_\lambda^{ab} = -\frac{m_a^2}{m_b} L^{ab} \frac{\partial \varphi_{b1}}{\partial \lambda}$$
(B.99)

$$F_{\lambda}^{ab} = -\frac{m_a^2}{m_b} L^{ab} \frac{\partial \varphi_{b1}}{\partial \lambda}$$
 (B.100)

$$F_{\varphi}^{ab} = -\frac{m_a^2}{m_b} L^{ab} \frac{\partial \varphi_{b1}}{\partial \varphi}. \tag{B.101}$$

Using Eqs. (B.95)-(B.97) and (B.99)-(B.101) and bearing Eq. (B.34) in mind the covariant components of collision flux in (v, λ, φ) coordinates become

$$j_{v}^{ab} = \frac{f_{a0}}{m_{a}} F_{v}^{ab} - (\mathbf{D} \cdot \nabla f_{a0})_{v}$$

$$= -L^{ab} f_{a0} \left(\frac{m_{a}}{m_{b}} \frac{\partial \varphi_{b1}}{\partial v} + \frac{2v}{v_{ta}^{2}} \frac{\partial^{2} \psi_{b1}}{\partial v^{2}} \right)$$

$$= \int_{\lambda}^{ab} F_{\lambda}^{ab} - (\mathbf{D} \cdot \nabla f_{a0})_{\lambda}$$

$$= -L^{ab} f_{a0} \left[\frac{m_{a}}{m_{b}} \frac{\partial \varphi_{b1}}{\partial \lambda} + \frac{2v}{v_{ta}^{2}} \left(\frac{\partial^{2} \psi_{b1}}{\partial \lambda \partial v} - \frac{1}{v} \frac{\partial \psi_{b1}}{\partial \lambda} \right) \right]$$

$$= \int_{\varphi}^{ab} F_{\varphi}^{ab} - (\mathbf{D} \cdot \nabla f_{a0})_{\varphi}$$

$$= -L^{ab} f_{a0} \left[\frac{m_{a}}{m_{b}} \frac{\partial \varphi_{b1}}{\partial \varphi} + \frac{2v}{v_{ta}^{2}} \left(\frac{\partial^{2} \psi_{b1}}{\partial \varphi \partial v} - \frac{1}{v} \frac{\partial \psi_{b1}}{\partial \varphi} \right) \right].$$
(B.104)

These components can now be substituted into Eq. (B.33) yielding

$$\mathcal{C}_{ab}[f_{a0}, f_{b1}] = -\frac{1}{\sqrt{g}} \frac{\partial}{\partial \xi^{i}} \left(\sqrt{g} g^{ik} j_{k}^{ab} \right) \\
= -\frac{1}{\sqrt{g}} \left[\frac{\partial}{\partial \xi^{1}} \left(\sqrt{g} g^{1k} j_{k}^{ab} \right) + \frac{\partial}{\partial \xi^{2}} \left(\sqrt{g} g^{2k} j_{k}^{ab} \right) + \frac{\partial}{\partial \xi^{3}} \left(\sqrt{g} g^{3k} j_{k}^{ab} \right) \right] \\
= -\frac{1}{\sqrt{g}} \left[\frac{\partial}{\partial \xi^{1}} \left(\sqrt{g} g^{11} j_{1}^{ab} \right) + \frac{\partial}{\partial \xi^{2}} \left(\sqrt{g} g^{22} j_{2}^{ab} \right) + \frac{\partial}{\partial \xi^{3}} \left(\sqrt{g} g^{33} j_{3}^{ab} \right) \right] \\
= -\frac{1}{v^{2}} \left[\frac{\partial}{\partial v} \left(v^{2} j_{v}^{ab} \right) + \frac{\partial}{\partial \lambda} \left((1 - \lambda^{2}) j_{\lambda}^{ab} \right) + \frac{\partial}{\partial \varphi} \left(\frac{j_{\varphi}^{ab}}{1 - \lambda^{2}} \right) \right] \\
= L^{ab} f_{a0} \left[-\frac{m_{a}}{m_{b}} \frac{2v}{v_{ta}^{2}} \frac{\partial \varphi_{b1}}{\partial v} + \frac{m_{a}}{m_{b} v^{2}} \frac{\partial}{\partial v} \left(v^{2} \frac{\partial \varphi_{b1}}{\partial v} \right) - \frac{4v^{2}}{v_{ta}^{2}} \frac{\partial^{2} \psi_{b1}}{\partial v^{2}} \right) \\
+ \frac{1}{v^{2}} \frac{\partial}{\partial v} \left(\frac{2v^{3}}{v_{ta}^{2}} \frac{\partial^{2} \psi_{b1}}{\partial v^{2}} \right) + \frac{m_{a}}{m_{b} v^{2}} \frac{\partial}{\partial \lambda} \left(1 - \lambda^{2} \right) \frac{\partial \varphi_{b1}}{\partial \lambda} \right]$$

$$+\frac{2v}{v_{ta}^{2}v^{2}}\frac{\partial}{\partial v}\frac{\partial}{\partial \lambda}\left(1-\lambda^{2}\right)\frac{\partial\psi_{b1}}{\partial \lambda}-\frac{2}{v_{ta}^{2}v^{2}}\frac{\partial}{\partial \lambda}\left(1-\lambda^{2}\right)\frac{\partial\psi_{b1}}{\partial \lambda}$$

$$+\frac{m_{a}}{m_{b}v^{2}(1-\lambda^{2})}\frac{\partial^{2}\varphi_{b1}}{\partial \varphi^{2}}+\frac{2v}{v_{ta}^{2}v^{2}(1-\lambda^{2})}\frac{\partial}{\partial v}\frac{\partial^{2}\psi_{b1}}{\partial \varphi^{2}}$$

$$-\frac{2}{v_{ta}^{2}v^{2}(1-\lambda^{2})}\frac{\partial^{2}\psi_{b1}}{\partial \varphi^{2}}\right].$$
(B.105)

Remembering the fact that the Trubnikov potentials satisfy Poisson's equation [see Eqs. (B.28) and (B.29)] and applying the Laplacian in spherical velocity-space coordinates to these equations one gets

$$f_{b1} = \nabla^{2}\varphi_{b1}$$

$$= \frac{1}{v^{2}} \left[\frac{\partial}{\partial v} \left(v^{2} \frac{\partial \varphi_{b1}}{\partial v} \right) + \frac{\partial}{\partial \lambda} (1 - \lambda^{2}) \frac{\partial \varphi_{b1}}{\partial \lambda} + \frac{1}{(1 - \lambda^{2})} \frac{\partial^{2}\varphi_{b1}}{\partial \varphi^{2}} \right] \quad (B.106)$$

$$\varphi_{b1} = \nabla^{2}\psi_{b1}$$

$$= \frac{1}{v^{2}} \left[\frac{\partial}{\partial v} \left(v^{2} \frac{\partial \psi_{b1}}{\partial v} \right) + \frac{\partial}{\partial \lambda} (1 - \lambda^{2}) \frac{\partial \psi_{b1}}{\partial \lambda} + \frac{1}{(1 - \lambda^{2})} \frac{\partial^{2}\psi_{b1}}{\partial \varphi^{2}} \right] \quad (B.107)$$

Utilizing Eqs. (B.106) and (B.107) and after elementary manipulation of Eq. (B.105) the field particle part of the linearized Coulomb collision operator eventually becomes

$$C_{ab}[f_{a0}, f_{b1}] = L^{ab} f_{a0} \left[\frac{m_a}{m_b} f_{b1} + \frac{2}{v_{ta}^2} \varphi_{b1} + \left(1 - \frac{m_a}{m_b} \right) \frac{2v}{v_{ta}^2} \frac{\partial \varphi_{b1}}{\partial v} - \frac{4v^2}{v_{ta}^4} \frac{\partial^2 \psi_{b1}}{\partial v^2} \right].$$
(B.108)

Appendix C

Trubnikov potentials for a non-Maxwellian distribution function f_{b1} in the Burnett basis

This appendix considers the evaluation of the Trubnikov potentials of the non-Maxwellian distribution function of the background particles in the Burnett function basis [81]. Due to Trubnikov [58] (see Appendix B.2 and also Reference 89) these functionals are represented as follows

$$\varphi_{b1}(\mathbf{v}) = -\frac{1}{4\pi} \int d^3 v' \frac{f_{b1}(\mathbf{v}')}{u(\mathbf{v}, \mathbf{v}')}$$
 (C.1)

$$\psi_{b1}(\mathbf{v}) = -\frac{1}{8\pi} \int d^3 v' u(\mathbf{v}, \mathbf{v}') f_{b1}(\mathbf{v}'), \qquad (C.2)$$

where the vector $\mathbf{u} = \mathbf{v} - \mathbf{v}'$ has been defined [22].

The expansion of the perturbation of the background distribution function f_{b1} in terms of Burnett functions $B_n^{(\ell)} = y^{\ell} L_n^{(\ell+1/2)}(y^2) P_{\ell}(\lambda)$ can be written as

$$f_{b1}(\mathbf{y}) = f_{b0}(y) \sum_{n=0}^{\infty} \sum_{\ell=0}^{\infty} \beta_n^{(\ell)} B_n^{(\ell)}(\mathbf{y}),$$
 (C.3)

with the Maxwellian

$$f_{b0}(y) = \frac{n_b}{\pi^{3/2} v_{tb}^3} e^{-y^2},$$
 (C.4)

and where the normalized velocity $\mathbf{y} = \mathbf{v}/v_{tb}$ has been used. When the Eq. (C.3) is substituted into Eqs. (C.1) and (C.2) one gets

$$\varphi_{b1}(\mathbf{y}) = \sum_{n=0}^{\infty} \sum_{\ell=0}^{\infty} \beta_n^{(\ell)} \Phi_n^{(\ell)}(\mathbf{y})$$
 (C.5)

$$\psi_{b1}(\mathbf{y}) = \sum_{n=0}^{\infty} \sum_{\ell=0}^{\infty} \beta_n^{(\ell)} \Psi_n^{(\ell)}(\mathbf{y}), \tag{C.6}$$

where the definitions

$$\Phi_n^{(\ell)} \equiv -\frac{1}{4\pi v_{tb}} \int d^3 v' \frac{f_{b0}(y')}{u(\mathbf{y}, \mathbf{y}')} B_n^{(\ell)}(\mathbf{y}')$$
 (C.7)

$$\Psi_n^{(\ell)} \equiv -\frac{v_{tb}}{8\pi} \int d^3 v' u(\mathbf{y}, \mathbf{y}') f_{b0}(y') B_n^{(\ell)}(\mathbf{y}')$$
 (C.8)

have been introduced.

As in conventional potential theory the functions $|\mathbf{y} - \mathbf{y}'|^{-1}$ and $|\mathbf{y} - \mathbf{y}'|$ may be expanded as a superposition of spherical harmonics which can be replaced by Legendre polynomials if azimuthal symmetry is assumed. Therefore, one has (see, e.g., Reference 92)

$$\overline{u^{-1}} = \sum_{k=0}^{\infty} \frac{y_{<}^k}{y_{>}^{k+1}} P_k(\lambda) P_k(\lambda'), \tag{C.9}$$

where $y_{<}(y_{>})$ is the smaller (larger) of $|\mathbf{y}|$ and $|\mathbf{y}'|$. In Appendix D the calculation of $|\mathbf{y} - \mathbf{y}'|$ is shown in detail yielding the result

$$\overline{u} = \sum_{k=0}^{\infty} \kappa^{(k)} (y_{<}, y_{>}) P_k(\lambda) P_k(\lambda'), \qquad (C.10)$$

where

$$\kappa^{(k)}(y_{<},y_{>}) = \frac{1}{(2k+3)} \frac{y_{<}^{k+2}}{y_{>}^{k+1}} - \frac{1}{(2k-1)} \frac{y_{<}^{k}}{y_{>}^{k-1}}.$$
 (C.11)

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Taking into account the volume element in spherical velocity-space coordinates, $d^3v = v^2dvd\lambda d\varphi$, Eq. (C.7) can be rewritten as

$$\Phi_n^{(\ell)}(\mathbf{y}) = -\frac{1}{4\pi v_{tb}} \int_0^{2\pi} d\varphi' \int_{-1}^1 d\lambda' \int_0^{\infty} dv' v'^2 \frac{1}{u(\mathbf{y}, \mathbf{y}')}$$

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$$\times y'^{\ell} L_n^{(\ell+1/2)}(y'^2) P_{\ell}(\lambda') \frac{n_b}{\pi^{3/2} v_{tb}^3} e^{-y'^2}$$

$$= -\frac{n_b}{2\pi^{3/2} v_{tb}} \int_{-1}^1 d\lambda' P_{\ell}(\lambda') \int_0^\infty dy' e^{-y'^2} y'^{\ell+2}$$

$$\times L_n^{(\ell+1/2)}(y'^2) \overline{u^{-1}}.$$
(C.12)

Substituting Eq. (C.9) into Eq. (C.12) one obtains

$$\Phi_{n}^{(\ell)}(\mathbf{y}) = -\frac{n_{b}}{2\pi^{3/2}v_{tb}} \int_{0}^{\infty} dy' e^{-y'^{2}} y'^{\ell+2} L_{n}^{(\ell+1/2)}(y'^{2})
\times \sum_{k=0}^{\infty} \frac{y_{<}^{k}}{y_{>}^{k+1}} P_{k}(\lambda) \int_{-1}^{1} d\lambda' P_{k}(\lambda') P_{\ell}(\lambda')
= -\frac{n_{b} P_{\ell}(\lambda)}{2\pi^{3/2}v_{tb}} \frac{2}{2\ell+1} \int_{0}^{\infty} dy' e^{-y'^{2}} y'^{\ell+2} L_{n}^{(\ell+1/2)}(y'^{2}) \frac{y_{<}^{\ell}}{y_{<}^{\ell+1}}, \quad (C.14)$$

where the orthogonality of the Legendre polynomials [29]

$$\int_{-1}^{1} d\lambda P_{\ell}(\lambda) P_{\ell'}(\lambda) = \frac{2}{2\ell + 1} \delta_{\ell\ell'}$$
 (C.15)

has been used. Therefore, Eq. (C.14) can be written as

$$\Phi_n^{(\ell)}(\mathbf{y}) = -\frac{n_b P_\ell(\lambda)}{2\pi^{3/2} v_{tb}} \hat{\varphi}_n^{(\ell)}(y), \tag{C.16}$$

where the dimensionless quantity

$$\hat{\varphi}_{n}^{(\ell)} = \frac{1}{(\ell+1/2)} \left[\frac{1}{y^{\ell+1}} \int_{0}^{y} dy' e^{-y'^{2}} y'^{2\ell+2} L_{n}^{(\ell+1/2)}(y'^{2}) + y^{\ell} \int_{y}^{\infty} dy' e^{-y'^{2}} y' L_{n}^{(\ell+1/2)}(y'^{2}) \right]$$
(C.17)

remains to be calculated. In carrying out this last equation one may utilize the results of Reference 49. The following integrals have been obtained¹,

$$\int dt e^{-t} t^{\alpha} L_n^{(\alpha)}(t) = \begin{cases} \gamma(\alpha + 1, t) & \text{for } n = 0\\ \frac{1}{n} e^{-t} t^{\alpha + 1} L_{n-1}^{(\alpha + 1)}(t) & \text{for } n \ge 1 \end{cases}$$
(C.18)

¹with the help of the formulas

http://functions.wolfram.com/07.03.21.0008.01

http://functions.wolfram.com/07.21.16.0001.01

http://functions.wolfram.com/07.21.27.0001.01

and

$$\int dt e^{-t} L_n^{(\alpha)}(t) = -e^{-t} L_n^{(\alpha-1)}(t), \tag{C.19}$$

where γ is the incomplete gamma function. Applying these integrals to Eq. (C.17) yields for n = 0

$$\hat{\varphi}_0^{(\ell)} = \frac{\gamma(\ell+1/2, y^2)}{2y^{\ell+1}} \tag{C.20}$$

$$\frac{\partial \hat{\varphi}_0^{(\ell)}}{\partial y} = e^{-y^2} y^{\ell-1} - \frac{(\ell+1)}{2} \frac{\gamma(\ell+1/2, y^2)}{y^{\ell+2}}, \tag{C.21}$$

and for $n \geq 1$

$$\hat{\varphi}_n^{(\ell)} = \frac{1}{2n} e^{-y^2} y^{\ell} L_{n-1}^{(\ell+1/2)}(y^2) \tag{C.22}$$

$$\frac{\partial \hat{\varphi}_{n}^{(\ell)}}{\partial y} = e^{-y^{2}} y^{\ell-1} \left[L_{n}^{(\ell-1/2)}(y^{2}) - \frac{(\ell+1)}{2n} L_{n-1}^{(\ell+1/2)}(y^{2}) \right]
= 2n \hat{\varphi}_{n}^{(\ell-1)} - \frac{(\ell+1)}{y} \hat{\varphi}_{n}^{(\ell)},$$
(C.23)

respectively. Using Eqs. (C.20) and (C.22), Eq. (C.21) can be rewritten to give

$$\frac{\partial \hat{\varphi}_0^{(\ell)}}{\partial y} = \frac{2}{y} \hat{\varphi}_1^{(\ell)} - \frac{(\ell+1)}{y} \hat{\varphi}_0^{(\ell)},\tag{C.24}$$

where $\hat{\varphi}_1^{(\ell-1)} = \hat{\varphi}_1^{(\ell)}/y$ has been applied.

Due to the fact that the incomplete gamma function as well as the associated Laguerre polynomials might be expressed in terms of the confluent hypergeometric function M(a, b, z) [47] (also called Kummer's function), that is

$$\gamma(\alpha, z) = \frac{z^{\alpha}}{\alpha} e^{-z} M(1, \alpha + 1, z)$$
 (C.25)

and

$$L_n^{(\alpha)}(z) = \binom{n+\alpha}{n} M(-n, \alpha+1, z), \tag{C.26}$$

with the binomial coefficient

$$\binom{n+\alpha}{n} = \frac{\Gamma(n+\alpha+1)}{n!\Gamma(\alpha+1)},\tag{C.27}$$

the dimensionless part of the first Trubnikov potential can also be presented as

$$\hat{\varphi}_n^{(\ell)} = \frac{\Gamma(n+\ell+1/2)}{2n!\Gamma(\ell+3/2)} y^{\ell} e^{-y^2} M(1-n,\ell+3/2,y^2) \quad \text{for} \quad n \ge 0. \quad (C.28)$$

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Hence, one finally obtains for the general solution of the first Trubnikov potential in terms of Burnett functions the following result

$$\Phi_n^{(\ell)} = -\frac{n_b P_\ell}{4\pi^{3/2} v_{tb}} \frac{\Gamma(n+\ell+1/2)}{n! \Gamma(\ell+3/2)} y^\ell e^{-y^2} M(1-n,\ell+3/2,y^2).$$
 (C.29)

For $n \geq 1$, this equation may also be expressed as $\Phi_n^{(\ell)} = -v_{tb}^2 f_{b0} B_{n-1}^{(\ell)}/(4n)$.

From the recurrence relations and differential properties for the confluent hypergeometric function one can derive corresponding expressions for the quantity $\hat{\varphi}_n^{(\ell)}$. After introducing the abbreviation

$$c_n^{(\ell)} \equiv \frac{\Gamma(n+\ell+1/2)}{2n!\Gamma(\ell+3/2)},$$
 (C.30)

one may express Eq. (C.28) as

$$\hat{\varphi}_n^{(\ell)} = c_n^{(\ell)} y^{\ell} e^{-y^2} M(1 - n, \ell + 3/2, y^2), \tag{C.31}$$

from which one can calculate the first derivative of $\hat{\varphi}_n^{(\ell)}$ with respect to y yielding

$$y\frac{\partial \hat{\varphi}_{n}^{(\ell)}}{\partial y} = yc_{n}^{(\ell)} \left[\frac{\partial}{\partial y} \left(y^{\ell} e^{-y^{2}} \right) M(1 - n, \ell + 3/2, y^{2}) \right]$$

$$+ y^{\ell} e^{-y^{2}} \frac{\partial}{\partial y} M(1 - n, \ell + 3/2, y^{2}) \right]$$

$$= c_{n}^{(\ell)} y^{\ell} e^{-y^{2}} \left\{ (\ell - 2y^{2}) M(1 - n, \ell + 3/2, y^{2}) - 2(n - 1) [M(2 - n, \ell + 3/2, y^{2}) - M(1 - n, \ell + 3/2, y^{2})] \right\}$$

$$= (\ell - 2y^{2}) \hat{\varphi}_{n}^{(\ell)} - \frac{(n + \ell - 1/2)}{n} 2(n - 1) \hat{\varphi}_{n-1}^{(\ell)} + 2(n - 1) \hat{\varphi}_{n}^{(\ell)}$$

$$= (2n + \ell - 2 - 2y^{2}) \hat{\varphi}_{n}^{(\ell)} - \frac{(n - 1)}{n} (2n + 2\ell - 1) \hat{\varphi}_{n-1}^{(\ell)}, \quad (C.32)$$

where the relations

$$y\frac{d}{dy}M(a,b,y^2) = 2y^2\frac{d}{dy^2}M(a,b,y^2)$$

= $2aM(a+1,b,y^2) - 2aM(a,b,y^2)$ (C.33)

(see, e.g., Reference 47) and, obtained from Eq. (C.30),

$$c_n^{(\ell)} = \frac{(n+\ell-1/2)}{n} c_{n-1}^{(\ell)} \tag{C.34}$$

have been applied. The recurrence relation [47]

$$aM(a+1,b,z) = (b-a)M(a-1,b,z) + (2a-b+z)M(a,b,z)$$
 (C.35)

vields

$$(n+\ell+1/2)M(-n,\ell+3/2,y^2) = (2n+\ell-1/2-y^2)M(1-n,\ell+3/2,y^2) - (n-1)M(2-n,\ell+3/2,y^2)$$
 (C.36)

from which one obtains upon multiplication of Eq. (C.36) by $c_n^{(\ell)} y^\ell e^{-y^2}$ (for $n \ge 1$)

$$(n+1)\hat{\varphi}_{n+1}^{(\ell)} = (2n+\ell-1/2-y^2)\hat{\varphi}_n^{(\ell)} - \frac{(n-1)}{n}(n+\ell-1/2)\hat{\varphi}_{n-1}^{(\ell)}.$$
 (C.37)

Substitution of Eq. (C.37) into Eq. (C.32) gives the result

$$y\frac{\partial \hat{\varphi}_n^{(\ell)}}{\partial y} = -(2n + \ell + 1)\hat{\varphi}_n^{(\ell)} + 2(n+1)\hat{\varphi}_{n+1}^{(\ell)} \quad \text{for} \quad n \ge 0.$$
 (C.38)

A relation with respect to the angular parameter ℓ can be calculated from Eq. (C.31) together with

$$c_n^{(\ell-1)} = \frac{(\ell+1/2)}{(n+\ell-1/2)} c_n^{(\ell)}$$
(C.39)

and Eq. (C.34), as well as the following recurrence formula for the Kummer function [47],

$$(b-1)M(a,b-1,z) = aM(a+1,b,z) - (a+1-b)M(a,b,z).$$
 (C.40)

One arrives at the expression

$$y\hat{\varphi}_n^{(\ell-1)} = \hat{\varphi}_n^{(\ell)} - \frac{(n-1)}{n}\hat{\varphi}_{n-1}^{(\ell)} \quad \text{for} \quad n \ge 1.$$
 (C.41)

Moreover, additional recurrence relations for the dimensionless first Trubnikov potential can be derived from the recurrence relations (see Eqs. 13.4.1-13.4.7 in Reference 47) for the confluent hypergeometric function M(a,b,z). These relations are as follows:

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$$y\hat{\varphi}_n^{(\ell)} = (n+\ell-1/2)\hat{\varphi}_n^{(\ell-1)} - (n+1)\hat{\varphi}_{n+1}^{(\ell-1)}$$
 (C.42)

$$y\hat{\varphi}_n^{(\ell+1)} = -(n+\ell-1/2)y\hat{\varphi}_n^{(\ell-1)} + (\ell+1/2+y^2)\hat{\varphi}_n^{(\ell)}$$
 (C.43)

$$(n+1)\hat{\varphi}_{n+1}^{(\ell)} = (n+\ell-1/2)y\hat{\varphi}_n^{(\ell-1)} + (n-y^2)\hat{\varphi}_n^{(\ell)}$$
 (C.44)

$$(n+1)y\hat{\varphi}_{n+1}^{(\ell-1)} = (\ell+1/2-y^2)\hat{\varphi}_n^{(\ell)} - \frac{(n-1)}{n}y\hat{\varphi}_{n-1}^{(\ell+1)}$$
 (C.45)

$$y\hat{\varphi}_n^{(\ell+1)} = (1-n+y^2)\hat{\varphi}_n^{(\ell)} + \frac{(n-1)}{n}(n+\ell-1/2)\hat{\varphi}_{n-1}^{(\ell)}(C.46)$$

$$y\hat{\varphi}_n^{(\ell+1)} = (\ell+1/2)\hat{\varphi}_n^{(\ell)} - (n+1)y\hat{\varphi}_{n+1}^{(\ell-1)}.$$
 (C.47)

$\mathbf{C.2}$ ψ_{b1}

According to Eq. (C.8) one obtains for the second Trubnikov potential

$$\Psi_{n}^{(\ell)}(\mathbf{y}) = -\frac{v_{tb}}{8\pi} \int_{0}^{2\pi} d\varphi' \int_{-1}^{1} d\lambda' \int_{0}^{\infty} dv' v'^{2} u(\mathbf{y}, \mathbf{y}')
\times y'^{\ell} L_{n}^{(\ell+1/2)}(y'^{2}) P_{\ell}(\lambda') \frac{n_{b}}{\pi^{3/2} v_{tb}^{3}} e^{-y'^{2}}
= -\frac{n_{b} v_{tb}}{4\pi^{3/2}} \int_{-1}^{1} d\lambda' P_{\ell}(\lambda') \int_{0}^{\infty} dy' e^{-y'^{2}} y'^{\ell+2}
\times L_{n}^{(\ell+1/2)}(y'^{2}) \overline{u}.$$
(C.48)

After substituting Eq. (C.10) into Eq. (C.48) it follows that

$$\Psi_{n}^{(\ell)} = -\frac{n_{b}v_{tb}}{4\pi^{3/2}} \int_{0}^{\infty} dy' e^{-y'^{2}} y'^{\ell+2} L_{n}^{(\ell+1/2)}(y'^{2})
\times \sum_{k=0}^{\infty} \kappa^{(k)} P_{k}(\lambda) \int_{-1}^{1} d\lambda' P_{\ell}(\lambda') P_{k}(\lambda')
= -\frac{n_{b}v_{tb}}{4\pi^{3/2}} P_{\ell}(\lambda) \frac{2}{2\ell+1} \int_{0}^{\infty} dy' e^{-y'^{2}} y'^{\ell+2} L_{n}^{(\ell+1/2)}(y'^{2}) \kappa^{(\ell)}, (C.49)$$

where Eq. (C.15) has been used. Hence, one may write

$$\Psi_n^{(\ell)}(\mathbf{y}) = -\frac{n_b v_{tb} P_\ell(\lambda)}{4\pi^{3/2}} \hat{\psi}_n^{(\ell)}(y), \tag{C.50}$$

where the dimensionless quantity

$$\hat{\psi}_{n}^{(\ell)} = \frac{1}{2(\ell+1/2)(\ell+3/2)} \left[\frac{1}{y^{\ell+1}} \int_{0}^{y} dy' e^{-y'^{2}} y'^{2\ell+4} L_{n}^{(\ell+1/2)}(y'^{2}) + y^{\ell+2} \int_{y}^{\infty} dy' e^{-y'^{2}} y' L_{n}^{(\ell+1/2)}(y'^{2}) \right]
- \frac{1}{2(\ell-1/2)(\ell+1/2)} \left[\frac{1}{y^{\ell-1}} \int_{0}^{y} dy' e^{-y'^{2}} y'^{2\ell+2} L_{n}^{(\ell+1/2)}(y'^{2}) + y^{\ell} \int_{y}^{\infty} dy' e^{-y'^{2}} y'^{3} L_{n}^{(\ell+1/2)}(y'^{2}) \right],$$
(C.51)

has been defined. This expression can be evaluated by recalling Eqs. (C.18) and (C.19), using [29]

$$L_n^{(\alpha)}(t) = L_n^{(\alpha+1)}(t) - L_{n-1}^{(\alpha+1)}(t), \tag{C.52}$$

performing an integration by parts and upon applying the recurrence relation for the incomplete gamma function [47]

$$\gamma(a+1,z) = a\gamma(a,z) - z^a e^{-z} \tag{C.53}$$

and further functional relations for the Laguerre polynomials [29]. One finally obtains for n = 0,

$$\hat{\psi}_0^{(\ell)} = \frac{1}{4} \left[\frac{\gamma(\ell+1/2, y^2)}{y^{\ell+1}} - \frac{\gamma(\ell-1/2, y^2)}{y^{\ell-1}} \right]$$
(C.54)

$$\frac{\partial^2 \hat{\psi}_0^{(\ell)}}{\partial y^2} = \frac{(\ell+1)(\ell+2)}{4} \frac{\gamma(\ell+1/2, y^2)}{y^{\ell+3}} - \frac{\ell(\ell-1)}{4} \frac{\gamma(\ell-1/2, y^2)}{y^{\ell+1}} - e^{-y^2} y^{\ell-2}, \quad (C.55)$$

for n=1,

$$\hat{\psi}_1^{(\ell)} = -\frac{\gamma(\ell+1/2, y^2)}{4u^{\ell+1}} \tag{C.56}$$

$$\frac{\partial^2 \hat{\psi}_1^{(\ell)}}{\partial y^2} = -\frac{(\ell+1)(\ell+2)}{4} \frac{\gamma(\ell+1/2, y^2)}{y^{\ell+3}} + e^{-y^2} \left(y^{\ell-2} + y^{\ell} \right), \quad (C.57)$$

and, finally, for $n \geq 2$

$$\hat{\psi}_n^{(\ell)} = -\frac{1}{4n(n-1)} e^{-y^2} y^{\ell} L_{n-2}^{(\ell+1/2)}(y^2)$$
 (C.58)

$$\frac{\partial^2 \hat{\psi}_n^{(\ell)}}{\partial y^2} = e^{-y^2} y^{\ell-2} \left[-\frac{(\ell+1)(\ell+2)}{4n(n-1)} L_{n-2}^{(\ell+1/2)}(y^2) + \frac{(2\ell+1)}{2n} L_{n-1}^{(\ell-1/2)}(y^2) - L_n^{(\ell-3/2)}(y^2) \right].$$
(C.59)

 $C.2. \ \psi_{B1}$ 185

Similar to the calculation of the function $\hat{\varphi}_n^{(\ell)}$ the quantity $\hat{\psi}_n^{(\ell)}$ can also be cast to a form which is valid for arbitrary n. Utilizing the equations [47]

$$M(1, b, z) = (b-1)\frac{e^z}{z^{b-1}}\gamma(b-1, z)$$
 (C.60)

$$M(2, b, z) = M(1, b, z) + z \frac{\partial}{\partial z} M(1, b, z)$$

= $(b-1)M(1, b-1, z) - (b-2)M(1, b, z)$, (C.61)

where the relation

$$z\frac{\mathrm{d}}{\mathrm{d}z}M(a,b,z) = (b-1)M(a,b-1,z) - (b-1)M(a,b,z) \tag{C.62}$$

has been applied [47, Eq. 13.4.13], the dimensionless part of the second Trubnikov potential can be presented as

$$\hat{\psi}_n^{(\ell)} = -\frac{\Gamma(n+\ell-1/2)}{4n!\Gamma(\ell+3/2)} y^{\ell} e^{-y^2} M(2-n,\ell+3/2,y^2) \quad \text{for} \quad n \ge 0, \quad (C.63)$$

from which one can infer that

$$\hat{\psi}_n^{(\ell)} = -\frac{1}{2n}\hat{\varphi}_{n-1}^{(\ell)} \quad \text{for} \quad n \ge 1,$$
 (C.64)

where Eq. (C.28) has been used. With the help of Eq. (C.41) one can find an additional representation for $\hat{\psi}_n^{(\ell)}$,

$$2(n-1)\hat{\psi}_n^{(\ell)} = y\hat{\varphi}_n^{(\ell-1)} - \hat{\varphi}_n^{(\ell)} \quad \text{for} \quad n \neq 1,$$
 (C.65)

from which one easily obtains the case for n=0,

$$\hat{\psi}_0^{(\ell)} = \frac{1}{2} \left[\hat{\varphi}_0^{(\ell)} - y \; \hat{\varphi}_0^{(\ell-1)} \right]. \tag{C.66}$$

Of course, the last equation could have also been derived from Eq. (C.54) and, furthermore, the mode $\hat{\varphi}_0^{(\ell-1)}$ might be evaluated from Eq. (C.44) by setting the lower index n equal to zero.

Using Eqs. (C.50) and (C.63) it follows that the general solution for the second Trubnikov potential in terms of Burnett functions may be written as

$$\Psi_n^{(\ell)}(\mathbf{y}) = \frac{n_b v_{tb} P_\ell(\lambda)}{16\pi^{3/2}} \frac{\Gamma(n+\ell-1/2)}{n! \Gamma(\ell+3/2)} y^\ell e^{-y^2} M(2-n,\ell+3/2,y^2).$$
 (C.67)

For $n \geq 2$, Eq. (C.67) can also be presented in the compact form $\Psi_n^{(\ell)} = v_{tb}^4 f_{b0} B_{n-2}^{(\ell)}/[16n(n-1)]$.

The derivatives of $\hat{\psi}_n^{(\ell)}$ with respect to the normalized speed y expressed in terms of the function $\hat{\varphi}_n^{(\ell)}$ readily follow from Eqs. (C.64) and (C.38), respectively, giving rise to

$$-2n\frac{\partial \hat{\psi}_{n}^{(\ell)}}{\partial y} = \frac{\partial \hat{\varphi}_{n-1}^{(\ell)}}{\partial y}$$
$$= \frac{1}{y} \left[2n\hat{\varphi}_{n}^{(\ell)} - (2n+\ell-1)\hat{\varphi}_{n-1}^{(\ell)} \right], \tag{C.68}$$

and

$$-2n\frac{\partial^{2}\hat{\psi}_{n}^{(\ell)}}{\partial y^{2}} = -\frac{1}{y^{2}} \left[2n\hat{\varphi}_{n}^{(\ell)} - (2n+\ell-1)\hat{\varphi}_{n-1}^{(\ell)} \right]$$

$$+\frac{1}{y^{2}} \left[2ny\frac{\partial\hat{\varphi}_{n}^{(\ell)}}{\partial y} - (2n+\ell-1)y\frac{\partial\hat{\varphi}_{n-1}^{(\ell)}}{\partial y} \right] , \quad (C.69)$$

and upon inserting of Eq. (C.68) into Eq. (C.69) it follows that

$$y^{2} \frac{\partial^{2} \hat{\psi}_{n}^{(\ell)}}{\partial y^{2}} = \hat{\varphi}_{n}^{(\ell)} - \frac{(2n+\ell-1)}{2n} \hat{\varphi}_{n-1}^{(\ell)} - \left[y \frac{\partial \hat{\varphi}_{n}^{(\ell)}}{\partial y} - \frac{(2n+\ell-1)}{2n} y \frac{\partial \hat{\varphi}_{n-1}^{(\ell)}}{\partial y} \right]$$

$$= \hat{\varphi}_{n}^{(\ell)} - \frac{(2n+\ell-1)}{2n} \hat{\varphi}_{n-1}^{(\ell)} - \left[2(n+1)\hat{\varphi}_{n+1}^{(\ell)} - (2n+\ell+1)\hat{\varphi}_{n}^{(\ell)} \right]$$

$$+ \frac{(2n+\ell-1)}{2n} \left[2n\hat{\varphi}_{n}^{(\ell)} - (2n+\ell-1)\hat{\varphi}_{n-1}^{(\ell)} \right]. \tag{C.70}$$

Hence, Eq. (C.70) can be simplified to give

$$y^{2} \frac{\partial^{2} \hat{\psi}_{n}^{(\ell)}}{\partial y^{2}} = -2(n+1)\hat{\varphi}_{n+1}^{(\ell)} + (4n+2\ell+1)\hat{\varphi}_{n}^{(\ell)} - \frac{(2n+\ell-1)}{2n}(2n+\ell)\hat{\varphi}_{n-1}^{(\ell)} \quad \text{for} \quad n \ge 1. \quad (C.71)$$

The case n=0 may be computed with the help of Eq. (C.55) yielding

$$y^{2} \frac{\partial^{2} \hat{\psi}_{0}^{(\ell)}}{\partial u^{2}} = \frac{(\ell+1)(\ell+2)}{2} \hat{\varphi}_{0}^{(\ell)} - \frac{\ell(\ell-1)}{2} y \hat{\varphi}_{0}^{(\ell-1)} - 2\hat{\varphi}_{1}^{(\ell)}. \tag{C.72}$$

C.3 Trubnikov potentials for a Maxwellian distribution function

For the case when the field particles are in thermodynamic equilibrium (Maxwellian background) the corresponding Trubnikov potentials may be

calculated from Eqs. (C.29) and (C.67), respectively, by setting the parameters n and ℓ equal to zero (and $\beta_0^0=1$). Thus, for the functional $\varphi_{b0} \equiv \Phi_0^{(0)}$ one obtains

$$\varphi_{b0}(y) = -\frac{n_b}{2\pi^{3/2}n_\mu}\hat{\varphi}_0^{(0)}(y), \tag{C.73}$$

with

$$\hat{\varphi}_0^{(0)} = \frac{\Gamma(1/2)}{2\Gamma(3/2)} e^{-y^2} M(1, 3/2, y^2)
= \frac{1}{2y} \gamma(1/2, y^2),$$
(C.74)

where Eq. (C.25) has been used and where $\gamma(\alpha, z)$ is the incomplete gamma function. Utilizing $\gamma(1/2, y^2) = \sqrt{\pi}\phi(y)$, where ϕ denotes the error function [47] one arrives at the expression

$$\varphi_{b0}(y) = -\frac{n_b}{4\pi v_{tb}} \frac{\phi(y)}{y}.$$
 (C.75)

The first derivative of the quantity φ_{b0} with respect to y follows immediately from the last equation, that is

$$\frac{\partial \varphi_{b0}}{\partial y} = -\frac{n_b}{4\pi v_{tb}} \frac{\partial}{\partial y} \left[\frac{\phi(y)}{y} \right]
= -\frac{n_b}{4\pi v_{tb}} \frac{\partial}{\partial y} \left(\frac{y\phi' - \phi}{y^2} \right).$$
(C.76)

Recalling the definition of the Chandrasekhar function, $G \equiv (\phi - y\phi')/(2y^2)$, Eq. (C.76) finally yields

$$\frac{\partial \varphi_{b0}}{\partial y} = \frac{n_b}{2\pi v_{tb}} G(y). \tag{C.77}$$

The second Trubnikov potential, $\psi_{b0} \equiv \Psi_0^{(0)}$, can be calculated in a similar way by using Eq. (C.63). It follows that

$$\psi_{b0}(y) = -\frac{n_b v_{tb}}{4\pi^{3/2}} \hat{\psi}_0^{(0)}(y), \tag{C.78}$$

with

$$\hat{\psi}_{0}^{(0)} = -\frac{\Gamma(-1/2)}{4\Gamma(3/2)}e^{-y^{2}}M(2,3/2,y^{2})$$

$$= -\frac{1}{4y}\left[y^{2}\gamma(-1/2,y^{2}) - \gamma(1/2,y^{2})\right]$$

$$= \frac{1}{2}\left[\sqrt{\pi}y\phi(y) + e^{-y^{2}} + \frac{\sqrt{\pi}}{2}\frac{\phi(y)}{y}\right].$$
(C.79)

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Applying Eqs. (C.60), (C.61) and (C.53) and again $\gamma(1/2, y^2) = \sqrt{\pi}\phi(y)$ gives

$$\psi_{b0}(v) = -\frac{n_b v_{tb}}{8\pi^{3/2}} \left[e^{-y^2} + \frac{\sqrt{\pi}}{2} \frac{\phi(y)}{y} + \sqrt{\pi} y \phi(y) \right]$$
$$= -\frac{n_b v_{tb}}{8\pi} \left[\frac{\phi'(y)}{2} + \frac{\phi(y)}{2y} + y \phi(y) \right], \tag{C.80}$$

where $\phi' \equiv d\phi/dy = 2e^{-y^2}/\sqrt{\pi}$ has been used.

The first derivative of ψ_{b0} with respect to normalized speed is readily obtained from Eq. (C.80),

$$\frac{\partial \psi_{b0}}{\partial y} = -\frac{n_b v_{tb}}{8\pi} \frac{\partial}{\partial y} \left[\frac{\phi'}{2} + \frac{\phi}{2y} + y\phi \right]
= -\frac{n_b v_{tb}}{8\pi} \left[\frac{\phi''}{2} + \frac{(y\phi' - \phi)}{2y^2} + \phi + y\phi' \right]
= \frac{n_b v_{tb}}{8\pi} \left[G(y) - \phi(y) \right],$$
(C.81)

where $\phi'' = -2y\phi'$ has been substituted. From Eq. (C.81) and the following relation for the derivative of the Chandrasekhar function G with respect to y,

$$G'(y) \equiv \frac{\mathrm{d}G(y)}{\mathrm{d}y} = \phi'(y) - \frac{2G(y)}{y},\tag{C.82}$$

one gets

$$\frac{\partial^2 \psi_{b0}}{\partial y^2} = \frac{n_b v_{tb}}{8\pi} \frac{\partial}{\partial y} \left[G(y) - \phi(y) \right] = -\frac{n_b v_{tb}}{4\pi} \frac{G(y)}{y}. \tag{C.83}$$

The functions $\partial \varphi_{b0}/\partial y$, $\partial \psi_{b0}/\partial y$ and $\partial^2 \psi_{b0}/\partial y^2$ appear during the derivation of the test particle collision operator $C_{ab}(f_{a1}, f_{b0})$ and are closely related to the three basic collision frequencies, namely the slowing down, the deflection and the parallel velocity diffusion frequency, respectively. A detailed description of the corresponding relationships has been given in Appendix (B.4.2).

Appendix D

Expansion of $|\mathbf{v} - \mathbf{v}'|$ in Legendre polynomials

In this Appendix the expansion of the absolute value of the relative velocity, $|\mathbf{v} - \mathbf{v}'|$, of colliding particles in Legendre polynomials is shown. The calculation utilizes the result for the corresponding expansion of the quantity $|\mathbf{v} - \mathbf{v}'|^{-1}$, which may be found in any textbook on electrodynamics (see, e.g., Reference 92).

The function $u \equiv |\mathbf{v} - \mathbf{v}'|$ is expanded in terms of Legendre polynomials P_k as

$$u(\alpha) = \sum_{k=0}^{\infty} a_k P_k(\alpha), \tag{D.1}$$

where $\alpha \equiv \cos \gamma$, and γ is the angle between the vectors \mathbf{v} and \mathbf{v}' . The expansion coefficients are given by

$$a_k = \frac{2k+1}{2} \int_{-1}^1 d\alpha u(\alpha) P_k(\alpha) = \frac{2k+1}{2} \int_{-1}^1 d\alpha \frac{u^2}{u} P_k(\alpha),$$
 (D.2)

wherein the function u^2 can be calculated to give

$$u^2 = v^2 + v'^2 - 2vv'\cos\gamma.$$
 (D.3)

In Eq. (D.2) the representation of the quantity 1/u in terms of Legendre polynomials is expressed as [92]

$$\frac{1}{u} = \sum_{k=0}^{\infty} \frac{v_{<}^{k}}{v_{>}^{k+1}} P_{k}(\alpha) , \qquad (D.4)$$

where $v_{<}(v_{>})$ is the smaller (larger) of $|\mathbf{v}|$ and $|\mathbf{v}'|$. Substituting Eqs. (D.3) and (D.4) into Eq. (D.2) yields

$$a_k = \frac{2k+1}{2} \sum_{k'=0}^{\infty} \frac{v_{<}^{k'}}{v_{>}^{k'+1}} \int_{-1}^{1} d\alpha P_{k'}(\alpha) \left(v_{<}^2 + v_{>}^2 - 2v_{<}v_{>}\alpha\right) P_k(\alpha).$$
 (D.5)

By virtue of the orthogonality of the Legendre polynomials [29],

$$\int_{-1}^{1} d\alpha P_{k'}(\alpha) P_k(\alpha) = \frac{2}{2k+1} \delta_{k'k}$$
 (D.6)

as well as the fact that the following integral vanishes unless $k' = k \pm 1$ [92],

$$\int_{-1}^{1} d\alpha \alpha P_{k'}(\alpha) P_{k}(\alpha) = \begin{cases}
\frac{2(k+1)}{(2k+1)(2k+3)} & \text{for } k' = k+1 \\
\frac{2k}{(2k-1)(2k+1)} & \text{for } k' = k-1
\end{cases}$$
(D.7)

one arrives at the following result for the expansion coefficients,

$$a_{k} = \frac{v_{<}^{k}}{v_{>}^{k+1}} \left(v_{<}^{2} + v_{>}^{2}\right) - \frac{v_{<}^{k+1}}{v_{>}^{k+2}} 2v_{<}v_{>} \frac{k+1}{2k+3} - \frac{v_{<}^{k-1}}{v_{>}^{k}} 2v_{<}v_{>} \frac{k}{2k-1}$$

$$= \frac{v_{<}^{k+2}}{v_{>}^{k+1}} \left(1 - \frac{2k+2}{2k+3}\right) + \frac{v_{<}^{k}}{v_{>}^{k-1}} \left(1 - \frac{2k}{2k-1}\right)$$

$$= \frac{v_{<}^{k+2}}{v_{>}^{k+1}} \frac{1}{(2k+3)} - \frac{v_{<}^{k}}{v_{>}^{k-1}} \frac{1}{(2k-1)}. \tag{D.8}$$

The angle γ can be expressed in terms of the spherical coordinates (θ, φ) and (θ', φ') , respectively, by the formula (the geometry is shown in Figure D.1)

$$\cos \gamma = \frac{\mathbf{v} \cdot \mathbf{v}'}{|\mathbf{v}||\mathbf{v}'|} = \cos \theta \cos \theta' + \sin \theta \sin \theta' \cos(\varphi - \varphi'). \tag{D.9}$$

The addition theorem for spherical harmonics [92] is a generalization of the last equation and states that

$$P_k(\cos \gamma) = P_k(\cos \theta) P_k(\cos \theta')$$

$$+ 2 \sum_{m=1}^k \frac{(k-m)!}{(k+m)!} P_k^m(\cos \theta) P_k^m(\cos \theta') \cos \left[m (\varphi - \varphi') \right], (D.10)$$

where P_k^m are called the associated Legendre functions [29].

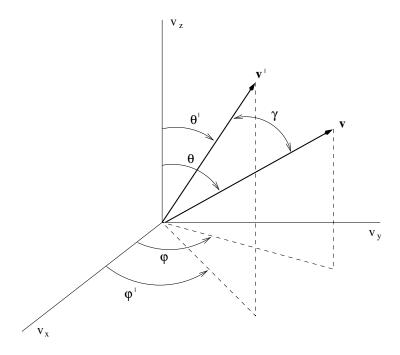


Figure D.1: Coordinates for the addition theorem for spherical harmonics.

In evaluating the Trubnikov potentials (see Appendix C) the functions u^{-1} and u might be replaced with $\overline{u^{-1}}$ and \overline{u} , respectively, where the overbar denotes the average over $(\varphi - \varphi')$ in spherical coordinates [82]. Thus, the desired expansions become

$$\overline{u^{-1}} = \sum_{k=0}^{\infty} \frac{v_{<}^{k}}{v_{>}^{k+1}} P_{k}(\cos \theta) P_{k}(\cos \theta') , \qquad (D.11)$$

and

$$\overline{u} = \sum_{k=0}^{\infty} \left[\frac{1}{(2k+3)} \frac{v_{<}^{k+2}}{v_{>}^{k+1}} - \frac{1}{(2k-1)} \frac{v_{<}^{k}}{v_{>}^{k-1}} \right] P_k(\cos\theta) P_k(\cos\theta'). \tag{D.12}$$

Appendix E

Braginskii matrix elements

In this appendix the Braginskii matrix elements [79] of the linearized Coulomb collision operator in terms of the so-called Burnett functions [81] are evaluated.

In contrast to earlier works [79, 80, 82] where the calculations were based upon the use of a generating function technique the method which is adopted here calculates directly the moments of the collision operator. Moreover, the obtained matrix elements are valid for arbitrary mass and temperature ratios. The results are compared to results given in References 79, 80, and 82 as well as to the results presented in Reference 90, which have also been obtained without using a generating function technique.

According to Braginskii [79] integrals of the form

$$\int d^3 v B_m^{(\ell)} \mathcal{C}_{ab} \left[f_{a0} B_{m'}^{(\ell)}, f_{b0} \right]$$
(E.1)

$$\int d^3 v B_m^{(\ell)} \mathcal{C}_{ab} \left[f_{a0}, B_{m'}^{(\ell)} f_{b0} \right]$$
(E.2)

are called matrix elements, where the quantities

$$B_m^{(\ell)}(x,\lambda) \equiv x^{\ell} L_m^{(\ell+1/2)}(x^2) P_{\ell}(\lambda)$$
 (E.3)

denote the Burnett functions. Here, $x = v/v_{ta}$, $y = v/v_{tb} = \gamma_{ab}x$, $\gamma_{ab} = v_{ta}/v_{tb}$, and $\lambda = v_{\parallel}/v$.

E.1 Linearized collision operator

When the gyrophase averaged guiding-center distribution functions of the test and field particles are assumed to be close to Maxwellian one can write

$$f_a = f_{a0} + f_{a1}$$
 (E.4)

$$f_b = f_{b0} + f_{b1},$$
 (E.5)

with f_{a0} , and f_{b0} being Maxwellians and f_{a1} , and f_{b1} representing small perturbations (that is $f_1 \ll f_0$) it is convenient to approximate the full Coulomb collision operator by its linearized form

$$C_{ab}[f_{a1}, f_{b1}] \approx C_{ab}[f_{a0}, f_{b0}] + C_{ab}[f_{a1}, f_{b0}] + C_{ab}[f_{a0}, f_{b1}], \tag{E.6}$$

in which the first term on the right-hand side of the last equation vanishes in the equal temperature case. The second term defines the test particle (or differential) part of the collision operator

$$C_{ab}[f_{a1}, f_{b0}] = \nu_D^{ab} \mathcal{L}[f_{a1}] + \frac{1}{v^2} \frac{\partial}{\partial v} \left[v^3 \left(\frac{m_a}{m_a + m_b} \nu_s^{ab} f_{a1} + \frac{v}{2} \nu_{\parallel}^{ab} \frac{\partial f_{a1}}{\partial v} \right) \right], \quad (E.7)$$

in which \mathcal{L} represents the pitch-angle scattering operator (for the case when the gyroangle φ can be ignored)

$$\mathcal{L} \equiv \frac{1}{2} \frac{\partial}{\partial \lambda} (1 - \lambda^2) \frac{\partial}{\partial \lambda}, \tag{E.8}$$

and the third term in Eq. (E.6) denotes the field particle (or integral) operator

$$\mathcal{C}_{ab}[f_{a0}, f_{b1}] = \frac{3n_a e^{-x^2}}{\tau_{ab} n_b} \left[\frac{m_a}{m_b} f_{b1} + \frac{2}{v_{ta}^2} \varphi_{b1} + \frac{2y}{v_{ta}^2} \left(1 - \frac{m_a}{m_b} \right) \frac{\partial \varphi_{b1}}{\partial y} - \frac{4y^2}{v_{ta}^4} \frac{\partial^2 \psi_{b1}}{\partial y^2} \right], \tag{E.9}$$

with the Trubnikov potentials φ_{b1} and ψ_{b1} being functionals of the field particle distribution f_{b1} (see Appendix C).

The following conservation laws [85,93] of the collision operator will be used to derive corresponding properties for the matrix elements.

The particle conservation is written as

$$\int d^3v \mathcal{C}_{ab} [f_{a1}, f_{b0}] = \int d^3v \mathcal{C}_{ab} [f_{a0}, f_{b1}] = 0,$$
 (E.10)

the momentum conservation reads

$$\int d^3 v m_a \mathbf{v} \mathcal{C}_{ab} \left[f_{a1}, f_{b0} \right] = - \int d^3 v m_b \mathbf{v} \mathcal{C}_{ba} \left[f_{b0}, f_{a1} \right], \tag{E.11}$$

and, finally, the energy conservation is expressed as

$$\int d^3v \frac{m_a v^2}{2} \mathcal{C}_{ab} [f_{a1}, f_{b0}] = -\int d^3v \frac{m_b v^2}{2} \mathcal{C}_{ba} [f_{b0}, f_{a1}].$$
 (E.12)

Furthermore, for equal species temperatures the differential and integral parts of the collision operator are self-adjoint [85,93], that is

$$\int d^3 v \frac{g_{a1}}{f_{a0}} \mathcal{C}_{ab} [f_{a1}, f_{b0}] = \int d^3 v \frac{f_{a1}}{f_{a0}} \mathcal{C}_{ab} [g_{a1}, f_{b0}], \qquad (E.13)$$

$$\int d^3v \frac{g_{a1}}{f_{a0}} \mathcal{C}_{ab} [f_{a0}, f_{b1}] = \int d^3v \frac{f_{b1}}{f_{b0}} \mathcal{C}_{ba} [f_{b0}, g_{a1}].$$
 (E.14)

E.2 Test particle part

The matrix elements of the differential part of the linearized collision operator are defined by

$$\mathsf{M}_{mm'}^{ab,(\ell)} \equiv \frac{\tau_{ab}}{n_a} \int d^3 v B_m^{(\ell)}(x,\lambda) \mathcal{C}_{ab} \left[f_{a0}(x) B_{m'}^{(\ell)}(x,\lambda), f_{b0}(y) \right]. \tag{E.15}$$

From Eq. (E.13) it follows that

$$\mathsf{M}_{mm'}^{ab,(\ell)} = \mathsf{M}_{m'm}^{ab,(\ell)}, \quad \text{for} \quad T_a = T_b.$$
 (E.16)

Introducing the volume element in spherical velocity-space coordinates, $d^3v = v^2 dv d\lambda d\varphi$ (see Appendix B.4.1), it follows that

$$\int d^3v = 2\pi v_{ta}^3 \int_{-1}^1 d\lambda \int_0^\infty dx x^2$$
 (E.17)

and one obtains from Eq. (E.15)

$$\mathsf{M}_{mm'}^{ab,(\ell)} = \frac{\tau_{ab}}{n_a} 2\pi v_{ta}^3 \int_{-1}^{1} \mathrm{d}\lambda \int_{0}^{\infty} \mathrm{d}x x^{\ell+2} L_m^{(\ell+1/2)} P_{\ell} \mathcal{C}_{ab} [f_{a0} x^{\ell} L_{m'}^{(\ell+1/2)} P_{\ell}, f_{b0}]$$

$$\equiv \nu_{mm'}^{ab,(\ell)} + D_{mm'}^{ab,(\ell)}. \tag{E.18}$$

The first part in Eq. (E.18) is related to the pitch-angle scattering operator whereas the second part corresponds to the energy scattering term of the

differential part of C_{ab} [see, Eq. (E.7)]. Taking into account that the Lorentz operator satisfies

$$\mathcal{L}[P_{\ell}(\lambda)] = -\frac{1}{2}\ell(\ell+1)P_{\ell}(\lambda), \tag{E.19}$$

it follows that

$$\nu_{mm'}^{ab,(\ell)} = \frac{\tau_{ab}}{n_a} 2\pi v_{ta}^3 \int_{-1}^{1} d\lambda \int_{0}^{\infty} dx x^{\ell+2} L_m^{(\ell+1/2)} P_{\ell} \nu_D^{ab} \mathcal{L}[f_{a0} x^{\ell} L_{m'}^{(\ell+1/2)} P_{\ell}]$$

$$= \frac{\tau_{ab}}{n_a} 2\pi v_{ta}^3 \int_{-1}^{1} d\lambda P_{\ell} \int_{0}^{\infty} dx x^{\ell+2} L_m^{(\ell+1/2)} \frac{3\sqrt{\pi}}{4\tau_{ab}} \frac{[\phi(y) - G(y)]}{x^3}$$

$$\times \frac{n_a e^{-x^2}}{\pi^{3/2} v_{ta}^3} x^{\ell} L_{m'}^{(\ell+1/2)} \mathcal{L}[P_{\ell}]$$

$$= -\frac{3\ell(\ell+1)}{2(2\ell+1)} \int_{0}^{\infty} dx e^{-x^2} x^{2\ell-1} L_m^{(\ell+1/2)} L_{m'}^{(\ell+1/2)} [\phi(y) - G(y)], \text{ (E.20)}$$

where the deflection frequency [22]

$$\nu_D^{ab}(v) = \frac{3\sqrt{\pi}}{4\tau_{ab}} \frac{[\phi(y) - G(y)]}{x^3}$$
 (E.21)

has been inserted and where the orthogonality relation of Legendre polynomials [29]

$$\int_{1}^{1} d\lambda P_{\ell}(\lambda) P_{\ell'}(\lambda) = \frac{2}{2\ell + 1} \delta_{\ell\ell'}$$
 (E.22)

has been applied. After replacing the Laguerre polynomials by its series representation (see, e.g., [29])

$$L_n^{(\alpha)}(z) = \sum_{j=0}^n \frac{(-1)^j}{j!} \binom{n+\alpha}{n-j} z^j,$$
 (E.23)

one obtains

$$\nu_{mm'}^{ab,(\ell)} = -\frac{3\ell(\ell+1)}{2(2\ell+1)} \sum_{j=0}^{m} \sum_{k=0}^{m'} S_{mm'}^{(\ell),jk} \int_{0}^{\infty} dx e^{-x^2} x^{2(j+k+\ell)-1} [\phi(y) - G(y)], \quad (E.24)$$

wherein

$$S_{mm'}^{(\ell),jk} = \frac{(-1)^{j+k}}{j!k!} {m+\ell+1/2 \choose m-j} {m'+\ell+1/2 \choose m'-k}.$$
 (E.25)

In evaluating Eq. (E.24) one must perform integrals of the form

$$\int_{0}^{\infty} dx e^{-x^{2}} x^{\alpha-1} \phi(y) = \frac{1}{\gamma^{\alpha}} \int_{0}^{\infty} dy e^{-y^{2}/\gamma^{2}} y^{\alpha-1} \frac{2y}{\sqrt{\pi}} e^{-y^{2}} M(1, 3/2, y^{2})$$

$$= \frac{2}{\sqrt{\pi} \gamma^{\alpha}} \int_{0}^{\infty} dy e^{-y^{2}(1+1/\gamma^{2})} y^{\alpha} M(1, 3/2, y^{2})$$

$$= \frac{1}{\sqrt{\pi} \gamma^{\alpha}} \int_{0}^{\infty} dt e^{-t(1+1/\gamma^{2})} t^{(\alpha-1)/2} M(1, 3/2, t)$$

$$= \frac{\Gamma(\frac{\alpha+1}{2})}{\sqrt{\pi}} \frac{\gamma}{(1+\gamma^{2})^{(\alpha+1)/2}} F(1, \frac{\alpha+1}{2}; \frac{3}{2}; \frac{\gamma^{2}}{1+\gamma^{2}}), (E.26)$$

where

$$\int_{0}^{\infty} dt e^{-st} t^{b-1} M(a, c, kt) = \frac{\Gamma(b)}{s^b} F(a, b; c; \frac{k}{s}), \quad \text{for} \quad |s| > |k| \quad (E.27)$$

has been used [29]. From the above results it follows that

$$\int_{0}^{\infty} dx e^{-x^{2}} x^{2(j+k+\ell)-1} \phi(y)$$

$$= \frac{\Gamma(j+k+\ell+1/2)\gamma}{\sqrt{\pi}(1+\gamma^{2})^{j+k+\ell+1/2}} F(1,j+k+\ell+\frac{1}{2};\frac{3}{2};\frac{\gamma^{2}}{1+\gamma^{2}}). \quad (E.28)$$

After performing an integration by parts applying

$$\int dy G(y) = -\frac{\phi(y)}{2y}, \qquad (E.29)$$

the integral corresponding to the term involving the Chandrasekhar function G in Eq. (E.24) can be reduced to integrals of the form Eq. (E.26), that is

$$\int_{0}^{\infty} dx e^{-x^{2}} x^{\alpha-1} G(y) = \frac{1}{\gamma^{\alpha}} \int_{0}^{\infty} dy e^{-y^{2}/\gamma^{2}} y^{\alpha-1} G(y)$$

$$= -\frac{1}{\gamma^{\alpha}} e^{-y^{2}/\gamma^{2}} y^{\alpha-1} \frac{\phi(y)}{2y} \Big|_{0}^{\infty}$$

$$+ \frac{1}{\gamma^{\alpha}} \int_{0}^{\infty} dy \frac{d}{dy} \left(e^{-y^{2}/\gamma^{2}} y^{\alpha-1} \right) \frac{\phi(y)}{2y}. \quad (E.30)$$

The first term in the last equation vanishes for the case when $\alpha \geq 2$. Substituting

$$\frac{\mathrm{d}}{\mathrm{d}y} \left(e^{-y^2/\gamma^2} y^{\alpha - 1} \right) = -\frac{2}{\gamma^2} y^{\alpha} e^{-y^2/\gamma^2} + (\alpha - 1) y^{\alpha - 2} e^{-y^2/\gamma^2} \tag{E.31}$$

into Eq. (E.30) the integral becomes (for $\alpha \geq 2$)

$$\int_{0}^{\infty} dx e^{-x^{2}} x^{\alpha-1} G(y) =$$

$$-\frac{1}{\gamma^{\alpha+2}} \int_{0}^{\infty} dy e^{-y^{2}/\gamma^{2}} y^{\alpha-1} \phi(y) + \frac{(\alpha-1)}{2\gamma^{\alpha}} \int_{0}^{\infty} dy e^{-y^{2}/\gamma^{2}} y^{\alpha-3} \phi(y)$$

$$= \frac{\Gamma(\frac{\alpha+1}{2})}{\sqrt{\pi} \gamma (1+\gamma^{2})^{(\alpha-1)/2}} \left[F(1, \frac{\alpha-1}{2}; \frac{3}{2}; \frac{\gamma^{2}}{1+\gamma^{2}}) - \frac{1}{(1+\gamma^{2})} F(1, \frac{\alpha+1}{2}; \frac{3}{2}; \frac{\gamma^{2}}{1+\gamma^{2}}) \right], \quad (E.32)$$

where the result of Eq. (E.26) has been used. Thus, for $(j + k + \ell) \ge 1$ one obtains

$$\int_{0}^{\infty} dx e^{-x^{2}} x^{2(j+k+\ell)-1} G(y) = \frac{\Gamma(j+k+\ell+1/2)}{\sqrt{\pi} \gamma (1+\gamma^{2})^{j+k+\ell+1/2}} \times \left[(1+\gamma^{2}) F(1,j+k+\ell-\frac{1}{2};\frac{3}{2};\frac{\gamma^{2}}{1+\gamma^{2}}) - F(1,j+k+\ell+\frac{1}{2};\frac{3}{2};\frac{\gamma^{2}}{1+\gamma^{2}}) \right]. \quad (E.33)$$

Combining Eqs. (E.28) and (E.33) one gets

$$\int_{0}^{\infty} dx e^{-x^{2}} x^{2(j+k+\ell)-1} \left[\phi(y) - G(y) \right] = \frac{\Gamma(j+k+\ell+1/2)}{\sqrt{\pi} \gamma (1+\gamma^{2})^{j+k+\ell-1/2}} \times \left[F(1,j+k+\ell+\frac{1}{2};\frac{3}{2};\frac{\gamma^{2}}{1+\gamma^{2}}) - F(1,j+k+\ell-\frac{1}{2};\frac{3}{2};\frac{\gamma^{2}}{1+\gamma^{2}}) \right]$$
(E.34)

and one finally obtains for the matrix elements of the pitch-angle scattering part of the collision operator

$$\nu_{mm'}^{ab,(\ell)}(\gamma) = \frac{3\ell(\ell+1)}{2(2\ell+1)} \sum_{j=0}^{m} \sum_{k=0}^{m'} S_{mm'}^{(\ell),jk} P_{\nu}^{(\ell),jk}(\gamma), \tag{E.35}$$

with $S_{mm'}^{(\ell),jk}$ given in Eq. (E.25) and

$$P_{\nu}^{(\ell),jk} = \frac{\Gamma(j+k+\ell+1/2)}{\sqrt{\pi}\gamma(1+\gamma^2)^{j+k+\ell-1/2}} \times \left[F(1,j+k+\ell-\frac{1}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) - F(1,j+k+\ell+\frac{1}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) \right]. \quad (E.36)$$

Recalling Eq. (E.18) the matrix elements corresponding to the energy scattering part of $C_{ab}[f_{a1}, f_{b0}]$ become

$$D_{mm'}^{ab,(\ell)} = \frac{\tau_{ab}}{n_a} 2\pi v_{ta}^3 \int_{-1}^{1} d\lambda \int_{0}^{\infty} dx x^{\ell+2} L_m^{(\ell+1/2)} P_{\ell} C_{ab}^{D} [f_{a0} x^{\ell} L_{m'}^{(\ell+1/2)} P_{\ell}]$$

$$= \frac{\tau_{ab}}{n_a} 2\pi \int_{-1}^{1} d\lambda P_{\ell} P_{\ell} \int_{0}^{\infty} dx x^{\ell+2} L_m^{(\ell+1/2)} \frac{1}{x^2} \frac{\partial}{\partial x} \left\{ \cdot \right\}, \quad (E.37)$$

where

$$\left\{ \cdot \right\} = v^{3} \left[\frac{\nu_{s}^{ab}}{(1 + m_{b}/m_{a})} f_{a0} x^{\ell} L_{m'}^{(\ell+1/2)} + \frac{\nu_{\parallel}^{ab}}{2} v \frac{\partial}{\partial v} \left(f_{a0} x^{\ell} L_{m'}^{(\ell+1/2)} \right) \right]. \quad (E.38)$$

The terms involving the slowing down frequency ν_s^{ab} , and the parallel velocity diffusion frequency ν_{\parallel}^{ab} , respectively, can be replaced by [22]

$$\frac{\nu_s^{ab}}{(1+m_b/m_a)} = \frac{3\sqrt{\pi}}{4\tau_{ab}} \frac{2T_a}{T_b} \frac{G(y)}{x}$$
 (E.39)

$$\frac{\nu_{\parallel}^{ab}}{2} = \frac{3\sqrt{\pi}}{4\tau_{ab}} \frac{G(y)}{x^3}, \tag{E.40}$$

and $\partial f_{a0}/\partial x = -2xf_{a0}$. From this and Eq. (E.22) it follows that

$$\begin{split} D_{mm'}^{ab,(\ell)} &= \frac{\pi^{3/2}}{n_a} \frac{3}{(2\ell+1)} \int\limits_0^\infty \mathrm{d}x x^\ell L_m^{(\ell+1/2)} \frac{\partial}{\partial x} \left[v^3 \frac{2T_a}{T_b} G(y) x^{\ell-1} \frac{n_a e^{-x^2}}{\pi^{3/2} v_{ta}^3} L_{m'}^{(\ell+1/2)} \right. \\ &\left. - v^3 \frac{G(y)}{x^2} \frac{n_a e^{-x^2}}{\pi^{3/2} v_{ta}^3} \left(2 x^{\ell+1} L_{m'}^{(\ell+1/2)} - \ell x^{\ell-1} L_{m'}^{(\ell+1/2)} - x^\ell \frac{\partial}{\partial x} L_{m'}^{(\ell+1/2)} \right) \right] \\ &= \frac{3}{(2\ell+1)} \int\limits_0^\infty \mathrm{d}x x^\ell L_m^{(\ell+1/2)} \frac{\partial}{\partial x} \left[\left(\frac{T_a}{T_b} - 1 \right) 2 x^{\ell+2} e^{-x^2} L_{m'}^{(\ell+1/2)} G(y) \right. \\ &\left. + \ell x^\ell e^{-x^2} L_{m'}^{(\ell+1/2)} G(y) + x^{\ell+1} e^{-x^2} \left(\frac{\partial}{\partial x} L_{m'}^{(\ell+1/2)} \right) G(y) \right] \end{split}$$

$$= \frac{3}{(2\ell+1)} \sum_{j=0}^{m} \sum_{k=0}^{m'} S_{mm'}^{(\ell),jk} \int_{0}^{\infty} dx x^{2j+\ell} \frac{\partial}{\partial x} \left[(2k+\ell)x^{2k+\ell} e^{-x^2} G(y) - \left(1 - \frac{T_a}{T_b} \right) 2x^{2k+\ell+2} e^{-x^2} G(y) \right].$$
 (E.41)

Performing an integration by parts one gets for the integral in Eq. (E.41)

$$\int_{0}^{\infty} dx x^{2j+\ell} \frac{\partial}{\partial x} \left[\cdot \right] = \left\{ x^{2j+\ell} \left[(2k+\ell) x^{2k+\ell} e^{-x^2} G(y) - \left(1 - \frac{T_a}{T_b} \right) 2x^{2k+\ell+2} e^{-x^2} G(y) \right] \right\} \Big|_{0}^{\infty} - (2j+\ell) \int_{0}^{\infty} dx x^{2j+\ell-1} \left[(2k+\ell) x^{2k+\ell} e^{-x^2} G(y) - \left(1 - \frac{T_a}{T_b} \right) 2x^{2k+\ell+2} e^{-x^2} G(y) \right] = -(2j+\ell)(2k+\ell) \int_{0}^{\infty} dx e^{-x^2} x^{2(j+k+\ell)-1} G(y) + (2j+\ell) \left(1 - \frac{T_a}{T_b} \right) 2 \int_{0}^{\infty} dx e^{-x^2} x^{2(j+k+\ell)+1} G(y), \tag{E.42}$$

where the integrals in the last equation can be carried out by using Eq. (E.32). Thus, one obtains for the energy scattering part of the test particle operator

$$D_{mm'}^{ab,(\ell)}(\gamma) = \frac{3}{(2\ell+1)} \sum_{j=0}^{m} \sum_{k=0}^{m'} S_{mm'}^{(\ell),jk} \times \left[P_{D1}^{(\ell),jk}(\gamma) + \left(1 - \frac{T_a}{T_b}\right) P_{D2}^{(\ell),jk}(\gamma) \right], \quad (E.43)$$

with

$$P_{D1}^{(\ell),jk}(\gamma) = -(2j+\ell)(2k+\ell)\frac{\Gamma(j+k+\ell+1/2)}{\sqrt{\pi}\gamma(1+\gamma^2)^{j+k+\ell+1/2}} \times \left[(1+\gamma^2)F(1,j+k+\ell-\frac{1}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) - F(1,j+k+\ell+\frac{1}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) \right]$$
(E.44)

$$P_{D2}^{(\ell),jk}(\gamma) = 2(2j+\ell)\frac{\Gamma(j+k+\ell+3/2)}{\sqrt{\pi}\gamma(1+\gamma^2)^{j+k+\ell+3/2}} \times \left[(1+\gamma^2)F(1,j+k+\ell+\frac{1}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) - F(1,j+k+\ell+\frac{3}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) \right] .$$
(E.45)

Putting Eqs. (E.35)-(E.36) and Eqs. (E.43)-(E.45) together one obtains for the matrix elements of the test particle operator in the Burnett basis

$$\mathsf{M}_{mm'}^{ab,(\ell)}(\gamma_{ab}) = \frac{3}{2\sqrt{\pi}\gamma_{ab}(2\ell+1)} \sum_{i=0}^{m+m'} \left[X_{mm'}^{(\ell),i} \, p_{\nu}^{(\ell),i}(\gamma_{ab}) - Y_{mm'}^{(\ell),i} \, p_{D}^{(\ell),i}(\gamma_{ab}) + \left(1 - \frac{T_a}{T_b} \right) Z_{mm'}^{(\ell),i} \, p_{D}^{(\ell),i+1}(\gamma_{ab}) \right], \tag{E.46}$$

where

$$X_{mm'}^{(\ell),i} = \ell(\ell+1) \sum_{j=0}^{i} S_{mm'}^{(\ell),ji-j}$$
 (E.47)

$$Y_{mm'}^{(\ell),i} = 2\sum_{j=0}^{i} S_{mm'}^{(\ell),ji-j} (2j+\ell)(2i-2j+\ell)$$
 (E.48)

$$Z_{mm'}^{(\ell),i} = 4 \sum_{j=0}^{i} S_{mm'}^{(\ell),ji-j} (2j+\ell),$$
 (E.49)

and

$$p_{\nu}^{(\ell),i}(\gamma) = \frac{\Gamma(i+\ell+1/2)}{(1+\gamma^2)^{i+\ell-1/2}} \times \left[F(1,i+\ell-\frac{1}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) - F(1,i+\ell+\frac{1}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) \right]$$
(E.50)
$$p_D^{(\ell),i}(\gamma) = \frac{\Gamma(i+\ell+1/2)}{(1+\gamma^2)^{i+\ell+1/2}} \times \left[(1+\gamma^2)F(1,i+\ell-\frac{1}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) - F(1,i+\ell+\frac{1}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) \right].$$
(E.51)

Noting that $S_{mm'}^{(\ell),jj}=S_{m'm}^{(\ell),jj},\,S_{mm'}^{(\ell),jk}=S_{m'm}^{(\ell),kj}$ and using the fact that $S_{mm'}^{(\ell),jk}=0$ for the case when j>m or k>m', one can show that $X_{mm'}^{(\ell),i}=X_{m'm}^{(\ell),i}$ and $Y_{mm'}^{(\ell),i}=Y_{m'm}^{(\ell),i}$, respectively. From this it follows that for $T_a=T_b$ the matrix elements $\mathsf{M}_{mm'}^{ab,(\ell)}$ satisfy the symmetry property Eq. (E.16), that is

$$\mathsf{M}_{mm'}^{ab,(\ell)}(\gamma_{ab}) = \mathsf{M}_{m'm}^{ab,(\ell)}(\gamma_{ab}).$$
 (E.52)

E.3 Field particle part

The matrix elements of the integral (momentum conserving) part of the linearized collision operator are defined by

$$N_{mm'}^{ab,(\ell)} \equiv \frac{\tau_{ab}}{n_a} \int d^3 v B_m^{(\ell)}(x,\lambda) C_{ab} \left[f_{a0}(x), B_{m'}^{(\ell)}(y,\lambda) f_{b0}(y) \right].$$
 (E.53)

From the self-adjoint property of the collision operator, Eq. (E.14), it follows that

$$\mathsf{N}_{mm'}^{ab,(\ell)} = \frac{\tau_{ab}}{n_a} \int \mathrm{d}^3 v B_{m'}^{(\ell)}(y,\lambda) \mathcal{C}_{ba} \left[f_{b0}(y), B_m^{(\ell)}(x,\lambda) f_{a0}(x) \right]
= \frac{\tau_{ab}}{n_a} \frac{n_b}{\tau_{ba}} \mathsf{N}_{m'm}^{ba,(\ell)}.$$
(E.54)

Taking into account that

$$\frac{\tau_{ab}}{n_a} \frac{n_b}{\tau_{ba}} = \frac{T_a^2}{T_b^2} \gamma_{ba} \tag{E.55}$$

one obtains

$$\mathsf{N}_{mm'}^{ab,(\ell)} = \gamma_{ba} \mathsf{N}_{m'm}^{ba,(\ell)}, \quad \text{for} \quad T_a = T_b.$$
(E.56)

Using Eqs. (E.17) and (E.22), Eq. (E.53) becomes

$$\mathsf{N}_{mm'}^{ab,(\ell)} = \frac{\tau_{ab}}{n_a} 2\pi v_{ta}^3 \int_{-1}^1 \mathrm{d}\lambda \int_0^\infty \mathrm{d}x x^2 P_{\ell}(\lambda) x^{\ell} L_m^{(\ell+1/2)}(x^2) \\
\times \mathcal{C}_{ab} \left[f_{a0}(x), f_{b0}(y) P_{\ell}(\lambda) y^{\ell} L_{m'}^{(\ell+1/2)}(y^2) \right] \\
= \frac{\tau_{ab}}{n_a} \frac{4\pi v_{ta}^3}{(2\ell+1)} \int_0^\infty \mathrm{d}x x^{\ell+2} L_m^{(\ell+1/2)}(x^2) \frac{3n_a e^{-x^2}}{\pi^{3/2} \tau_{ab} v_{tb}^3 \gamma^4} \left\{ \cdot \right\}. \quad (E.57)$$

Provided $m' \geq 2$ the expression in the curly brackets reads

$$\left\{ \cdot \right\} = -(2m'+\ell)\frac{(2m'+\ell-1)}{2m'}\hat{\varphi}_{m'-1}^{(\ell)} + \left[(2m'+\ell+1)\left(1-\frac{T_a}{T_b}\right) + (2m'+\ell)\left(1+\gamma^2\right) \right]\hat{\varphi}_{m'}^{(\ell)} - 2(m'+1)\left(1+\gamma^2\right)\left(1-\frac{T_a}{T_b}\right)\hat{\varphi}_{m'+1}^{(\ell)}, (E.58)$$

where the main results of Appendix C have been substituted into Eq. (E.9). Thus, Eq. (E.57) can be expressed as

$$\mathsf{N}_{mm'}^{ab,(\ell)} \ = \ \frac{2}{\sqrt{\pi}} \frac{2}{(2\ell+1)} \frac{3}{\gamma} \left\{ -(2m'+\ell) \frac{(2m'+\ell-1)}{2m'} I_{mm'-1}^{(\ell)} \right\}$$

+
$$\left[(2m' + \ell + 1) \left(1 - \frac{T_a}{T_b} \right) + (2m' + \ell) \left(1 + \gamma^2 \right) \right] I_{mm'}^{(\ell)}$$

- $2(m' + 1) \left(1 + \gamma^2 \right) \left(1 - \frac{T_a}{T_b} \right) I_{mm'+1}^{(\ell)} \right\},$ (E.59)

where the quantities $I_{mn}^{(\ell)}$ denote

$$I_{mn}^{(\ell)} \equiv \int_{0}^{\infty} dx e^{-x^{2}} x^{\ell+2} L_{m}^{(\ell+1/2)}(x^{2}) \hat{\varphi}_{n}^{(\ell)}(y), \qquad (E.60)$$

and wherein the quantity $\hat{\varphi}_n^{(\ell)}$ is related to the first Trubnikov potential (see Appendix C.1),

$$\hat{\varphi}_n^{(\ell)}(y) = \frac{1}{2n} e^{-y^2} y^{\ell} L_{n-1}^{(\ell+1/2)}(y^2), \quad \text{for} \quad n \ge 1.$$
 (E.61)

Using $y = \gamma x$ one obtains

$$I_{mn}^{(\ell)} = \frac{1}{\gamma^{\ell+3}} \int_{0}^{\infty} \mathrm{d}y e^{-y^{2}/\gamma^{2}} y^{\ell+2} L_{m}^{(\ell+1/2)}(y^{2}/\gamma^{2}) \frac{1}{2n} e^{-y^{2}} y^{\ell} L_{n-1}^{(\ell+1/2)}(y^{2})$$

$$= \frac{1}{2n\gamma^{\ell+3}} \int_{0}^{\infty} \mathrm{d}y e^{-y^{2}(1+\gamma^{-2})} y^{2\ell+2} L_{m}^{(\ell+1/2)}(y^{2}/\gamma^{2}) L_{n-1}^{(\ell+1/2)}(y^{2})$$

$$= \frac{1}{4n\gamma^{\ell+3}} \int_{0}^{\infty} \mathrm{d}t e^{-t(1+\gamma^{-2})} t^{\ell+1/2} L_{m}^{(\ell+1/2)}(t/\gamma^{2}) L_{n-1}^{(\ell+1/2)}(t). \quad (E.62)$$

In the evaluation of Eq. (E.62) one may use the following formula (see, Reference 29),

$$\int_{0}^{\infty} dx e^{-x(\lambda+\mu)} x^{\alpha} L_{M}^{(\alpha)}(\lambda x) L_{N}^{(\alpha)}(\mu x) = \frac{\Gamma(M+N+\alpha+1)\mu^{M}\lambda^{N}}{M!N! (\lambda+\mu)^{M+N+\alpha+1}}, \quad (E.63)$$

provided that Re $\alpha > -1$, Re $\lambda + \mu > 0$, yielding

$$\int_{0}^{\infty} dt e^{-t(1+\gamma^{-2})} t^{\ell+1/2} L_{m}^{(\ell+1/2)}(t/\gamma^{2}) L_{n-1}^{(\ell+1/2)}(t) = \frac{\Gamma(m+n+\ell+1/2)\gamma^{2m+2\ell+3}}{m!(n-1)!(1+\gamma^{2})^{m+n+\ell+1/2}}.$$
(E.64)

Thus, the integral (E.60) has the result

$$I_{mn}^{(\ell)} = \frac{\Gamma(m+n+\ell+1/2)}{4m!n!} \frac{\gamma^{2m+\ell}}{(1+\gamma^2)^{m+n+\ell+1/2}}.$$
 (E.65)

Applying Eq. (E.65) to the corresponding terms in the curly brackets of Eq. (E.59) gives

$$(1+\gamma^{2}) I_{mm'}^{(\ell)} - \frac{(2m'+\ell-1)}{2m'} I_{mm'-1}^{(\ell)} = \frac{\Gamma(m+m'+\ell+1/2)\gamma^{2m+\ell}}{4m!m'!(1+\gamma^{2})^{m+m'+\ell-1/2}} - \frac{(2m'+\ell-1)}{2m'} \frac{\Gamma(m+m'+\ell-1/2)\gamma^{2m+\ell}}{4m!(m'-1)!(1+\gamma^{2})^{m+m'+\ell-1/2}} = \frac{\Gamma(m+m'+\ell-1/2)\gamma^{2m+\ell}}{4m!m'!(1+\gamma^{2})^{m+m'+\ell-1/2}} (m+\ell/2), \quad (E.66)$$

and

$$(2m'+\ell+1)I_{mm'}^{(\ell)} - 2(m'+1)\left(1+\gamma^{2}\right)I_{mm'+1}^{(\ell)} =$$

$$(2m'+\ell+1)\frac{\Gamma(m+m'+\ell+1/2)\gamma^{2m+\ell}}{4m!m'!(1+\gamma^{2})^{m+m'+\ell+1/2}}$$

$$-2(m'+1)\frac{\Gamma(m+m'+\ell+3/2)\gamma^{2m+\ell}}{4m!(m'+1)!(1+\gamma^{2})^{m+m'+\ell+1/2}}$$

$$= -\frac{\Gamma(m+m'+\ell+1/2)\gamma^{2m+\ell}}{4m!m'!(1+\gamma^{2})^{m+m'+\ell+1/2}}(2m+\ell), \quad (E.67)$$

respectively.

Substituting from Eqs. (E.66) and (E.67) into Eq. (E.59), one obtains for the matrix elements of the field particle operator in the Burnett basis

$$\begin{split} \mathsf{N}_{mm'}^{ab,(\ell)}(\gamma_{ab}) \; &= \; \frac{3}{2\sqrt{\pi}} \frac{(2m+\ell)}{(2\ell+1)} \frac{\Gamma(m+m'+\ell-1/2)}{m! \; m'!} \frac{\gamma_{ab}^{2m+\ell-1}}{(1+\gamma_{ab}^2)^{m+m'+\ell+1/2}} \\ & \times \; \left[(2m'+\ell)(1+\gamma_{ab}^2) - 2(m+m'+\ell-1/2) \left(1-\frac{T_a}{T_b}\right) \right]. \; \text{(E.68)} \end{split}$$

After simple but somewhat tedious calculations [involving Eq. (E.57) as well as Eqs. (C.20)-(C.23) and (C.55)-(C.57)] one can show that this result is also valid for m'=0 and 1, respectively. Here it is worth noting that, in contrast to the results for the test particle operator where the matrix elements have been expressed as finite sum of Gauss' hypergeometric functions [cf. Eqs. (E.46)-(E.51)], the matrix elements of the field particle operator, Eq. (E.68), have

been presented for the first time, to the author's knowledge, in a compact analytical form.

Assuming equal species temperatures, $T_a = T_b$, Eq. (E.68) yields

$$\mathsf{N}_{mm'}^{ab,(\ell)} = \frac{3}{2\sqrt{\pi}} \frac{(2m+\ell)(2m'+\ell)}{(2\ell+1)} \frac{\Gamma(m+m'+\ell-1/2)}{m! \ m'!} \frac{\gamma_{ab}^{2m+\ell-1}}{(1+\gamma_{ab}^2)^{m+m'+\ell-1/2}},\tag{E.69}$$

from which it follows that

$$\mathsf{N}_{m'm}^{ab,(\ell)}(\gamma_{ab}) = \gamma_{ab}^{2(m'-m)} \mathsf{N}_{mm'}^{ab,(\ell)}(\gamma_{ab}) \tag{E.70}$$

$$\mathsf{N}_{mm'}^{ba,(\ell)}(\gamma_{ba}) = \gamma_{ab} \mathsf{N}_{m'm}^{ab,(\ell)}(\gamma_{ab}). \tag{E.71}$$

Here, Eq. (E.71) demonstrates the self-adjointness of the field particle part of the collision operator [see Eq. (E.56)].

The matrix elements for the case when the test and field particle distribution functions are Maxwellians at different temperatures can easily be calculated from Eqs. (E.46) or (E.68), respectively, using m' = 0 and $\ell = 0$. One finds that

$$\mathsf{M}_{m0}^{ab,(0)} = \mathsf{N}_{m0}^{ab,(0)} = -\frac{6}{\sqrt{\pi}} \frac{m\Gamma(m+1/2)}{m!} \frac{\gamma_{ab}^{2m-1}}{(1+\gamma_{ab}^2)^{m+1/2}} \left(1 - \frac{T_a}{T_b}\right). \quad (E.72)$$

E.4 Conservation laws

In this section it is shown that the matrix elements of the linearized collision operator calculated above satisfy the properties that can be derived from the conservation laws of the collision operator.

E.4.1 Particle conservation

In view of Eqs. (E.10), (E.15) and (E.53), and with $1 = B_0^{(0)}$ one has

$$\mathsf{M}_{0m'}^{ab,(0)}(\gamma_{ab}) = \mathsf{N}_{0m'}^{ab,(0)}(\gamma_{ab}) = 0 \tag{E.73}$$

which follows directly from Eqs. (E.46)-(E.49) and Eq. (E.68), respectively.

E.4.2 Momentum conservation

By making use of Eq. (E.11) one can derive

$$\frac{T_a}{v_{ta}} \int d^3v x \lambda \mathcal{C}_{ab} \left[f_{a1}, f_{b0} \right] = -\frac{T_b}{v_{tb}} \int d^3v y \lambda \mathcal{C}_{ba} \left[f_{b0}, f_{a1} \right]$$
 (E.74)

and with the help of Eqs. (E.15) and (E.53) one obtains

$$\frac{T_a}{v_{ta}} \frac{n_a}{\tau_{ab}} \mathsf{M}_{0m'}^{ab,(1)}(\gamma_{ab}) = -\frac{T_b}{v_{tb}} \frac{n_b}{\tau_{ba}} \mathsf{N}_{0m'}^{ba,(1)}(\gamma_{ba}) \tag{E.75}$$

which finally yields

$$\mathsf{M}_{0m'}^{ab,(1)}(\gamma_{ab}) = -\frac{T_a}{T_b} \mathsf{N}_{0m'}^{ba,(1)}(\gamma_{ba}), \tag{E.76}$$

where Eq. (E.55) has been used. The matrix elements on the right-hand side of the last equation reads [cf. Eq. (E.68)],

$$\mathsf{N}_{0m'}^{ba,(1)}(\gamma_{ba}) = \frac{\Gamma(m'+3/2)}{\sqrt{\pi}m'!(1+\gamma_{ba}^2)^{m'+3/2}} \left[(1+\gamma_{ba}^2) - \left(1-\frac{T_b}{T_a}\right) \right]. \tag{E.77}$$

Recalling Eqs. (E.46)-(E.51) one obtains for m=0 and $\ell=1$,

$$\mathsf{M}_{0m'}^{ab,(1)}(\gamma_{ab}) = \frac{1}{2\sqrt{\pi}\gamma_{ab}} \sum_{i=0}^{m} \left[X_{0m'}^{(1),i} \, p_{\nu}^{(1),i}(\gamma_{ab}) - Y_{0m'}^{(1),i} \, p_{D}^{(1),i}(\gamma_{ab}) + \left(1 - \frac{T_a}{T_b}\right) Z_{0m'}^{(1),i} \, p_{D}^{(1),i+1}(\gamma_{ab}) \right], \tag{E.78}$$

with

$$X_{0m'}^{(1),i} = 2\sum_{j=0}^{i} S_{0m'}^{(1),ji-j} = 2\frac{(-1)^{i}}{i!} {m'+3/2 \choose m'-i}$$
 (E.79)

$$Y_{0m'}^{(1),i} = 2\sum_{j=0}^{i} S_{0m'}^{(1),ji-j} (2j+1)(2i-2j+1)$$

$$= 2\frac{(-1)^{i}}{i!} {m'+3/2 \choose m'-i} (2i+1)$$
(E.80)

$$Z_{0m'}^{(1),i} = 4 \sum_{j=0}^{i} S_{0m'}^{(1),ji-j}(2j+1) = 4 \frac{(-1)^{i}}{i!} {m'+3/2 \choose m'-i},$$
 (E.81)

and

$$p_{\nu}^{(1),i}(\gamma) = \frac{\Gamma(i+3/2)}{(1+\gamma^2)^{i+1/2}} \left[F(1,i+\frac{1}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) - F(1,i+\frac{3}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) \right]$$
(E.82)
$$p_D^{(1),i}(\gamma) = \frac{\Gamma(i+3/2)}{(1+\gamma^2)^{i+1/2}} \left[F(1,i+\frac{1}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) - \frac{F(1,i+\frac{3}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2})}{(1+\gamma^2)} \right]$$
$$= \frac{\Gamma(i+1/2)}{2(1+\gamma^2)^{i+1/2}} \left[F(1,i+\frac{1}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) - 1 \right].$$
(E.83)

In Reference 47 one can find the following relation for the hypergeometric function F,

$$b(1-z)F(1,b+1;c;z) = (c-1) - (c-1-b)F(1,b;c;z),$$
 (E.84)

from which it follows that

$$\frac{(2i+2\ell-1)}{(1+\gamma^2)}F(1,i+\ell+\frac{1}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) = 1 + 2(i+\ell-1)F(1,i+\ell-\frac{1}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}). \quad (E.85)$$

Substituting Eqs. (E.79)- (E.83) and Eq. (E.85) into Eq. (E.78) one can show that

$$\mathsf{M}_{0m'}^{ab,(1)}(\gamma) = \frac{1}{\sqrt{\pi}\gamma} \sum_{i=0}^{m'} \frac{(-1)^i}{i!} {m'+3/2 \choose m'-i} \frac{\Gamma(i+3/2)}{(1+\gamma^2)^{i+1/2}} \times \left[1 - F(1, i + \frac{3}{2}; \frac{3}{2}; \frac{\gamma^2}{1+\gamma^2}) + \left(1 - \frac{T_a}{T_b}\right) \frac{F(1, i + \frac{3}{2}; \frac{3}{2}; \frac{\gamma^2}{1+\gamma^2}) - 1}{(1+\gamma^2)} \right]. \quad (E.86)$$

The following relations have been obtained by means of Maple [48],

$$\sum_{i=0}^{m'} \frac{(-1)^i}{i!} {m'+3/2 \choose m'-i} \frac{\Gamma(i+3/2)}{(1+\gamma^2)^i}
= \frac{\sqrt{\pi}}{2} {m'+3/2 \choose m'} F(-m', \frac{3}{2}; \frac{5}{2}; \frac{1}{1+\gamma^2}), \quad (E.87)$$

$$\sum_{i=0}^{m'} \frac{(-1)^i}{i!} {m'+3/2 \choose m'-i} \frac{\Gamma(i+3/2)}{(1+\gamma^2)^i} F(1, i+\frac{3}{2}; \frac{3}{2}; \frac{\gamma^2}{1+\gamma^2})$$

$$= \frac{\sqrt{\pi}}{2} (1+\gamma^2) {m'+1/2 \choose m'} F(-m', \frac{1}{2}; \frac{3}{2}; \frac{1}{1+\gamma^2}). \text{ (E.88)}$$

Therefore, one has

$$\mathsf{M}_{0m'}^{ab,(1)}(\gamma) = \frac{(1+\gamma^2)^{1/2}}{2\gamma} \left[\binom{m'+3/2}{m'} \frac{F(-m', \frac{3}{2}; \frac{5}{2}; \frac{1}{1+\gamma^2})}{(1+\gamma^2)} - \binom{m'+1/2}{m'} F(-m', \frac{1}{2}; \frac{3}{2}; \frac{1}{1+\gamma^2}) \right] + \left(1 - \frac{T_a}{T_b}\right) \frac{1}{2\gamma(1+\gamma^2)^{1/2}} \times \left[\binom{m'+1/2}{m'} F(-m', \frac{1}{2}; \frac{3}{2}; \frac{1}{1+\gamma^2}) - \binom{m'+3/2}{m'} \frac{F(-m', \frac{3}{2}; \frac{5}{2}; \frac{1}{1+\gamma^2})}{(1+\gamma^2)} \right] . (E.89)$$

With the help of the following formula [47],

$$c(1-z)F(a,b;c;z) = cF(a,b-1;c;z) - (c-a)zF(a,b;c+1;z), \quad (E.90)$$

one arrives at the relation

$$\frac{3}{2} \frac{\gamma^{2}}{(1+\gamma^{2})} F(-m', \frac{3}{2}; \frac{3}{2}; \frac{1}{1+\gamma^{2}}) = \frac{3}{2} F(-m', \frac{1}{2}; \frac{3}{2}; \frac{1}{1+\gamma^{2}}) - \frac{(m'+3/2)}{(1+\gamma^{2})} F(-m', \frac{3}{2}; \frac{5}{2}; \frac{1}{1+\gamma^{2}}). (E.91)$$

The hypergeometric function on the left-hand side of the last equation can be simplified to give

$$F(-m', \frac{3}{2}; \frac{3}{2}; \frac{1}{1+\gamma^2}) = \frac{\gamma^{2m'}}{(1+\gamma^2)^{m'}},$$
 (E.92)

where $F(a, b; b; z) = (1-z)^{-a}$ has been applied [47]. Thus, the matrix elements related to the first collisional moment of the differential operator read

$$\mathsf{M}_{0m'}^{ab,(1)}(\gamma_{ab}) = -\frac{\Gamma(m'+3/2)}{\sqrt{\pi}m'!} \frac{\gamma_{ab}^{2m'+1}}{(1+\gamma_{ab}^2)^{m'+1/2}} + \left(1 - \frac{T_a}{T_b}\right) \frac{\Gamma(m'+3/2)}{\sqrt{\pi}m'!} \frac{\gamma_{ab}^{2m'+1}}{(1+\gamma_{ab}^2)^{m'+3/2}} = -\frac{\Gamma(m'+3/2)\gamma_{ab}^{2m'+1}}{\sqrt{\pi}m'!(1+\gamma_{ab}^2)^{m'+3/2}} \left[(1+\gamma_{ab}^2) - \left(1 - \frac{T_a}{T_b}\right) \right]. (E.93)$$

The momentum conservation of particles can now be verified by replacing $\gamma_{ab} = 1/\gamma_{ba}$ in Eq. (E.93), that is

$$-\frac{T_b}{T_a} \mathsf{M}_{0m'}^{ab,(1)}(\gamma_{ba}) = \frac{\Gamma(m'+3/2)}{\sqrt{\pi}m'!(1+\gamma_{ba}^2)^{m'+3/2}} \left[\frac{T_b}{T_a} (1+\gamma_{ba}^2) - \left(\frac{T_b}{T_a} - 1\right) \gamma_{ba}^2 \right]$$
$$= \frac{\Gamma(m'+3/2)}{\sqrt{\pi}m'!(1+\gamma_{ba}^2)^{m'+3/2}} \left[1+\gamma_{ba}^2 - \left(1-\frac{T_b}{T_a}\right) \right], \quad (E.94)$$

which is in agreement with Eq. (E.77).

E.4.3 Energy conservation

From Eq. (E.12) one finds

$$T_a \int d^3v x^2 \mathcal{C}_{ab} [f_{a1}, f_{b0}] = -T_b \int d^3v y^2 \mathcal{C}_{ba} [f_{b0}, f_{a1}]$$
 (E.95)

After replacing x^2 and y^2 with $(3/2)B_0^{(0)} - B_1^{(0)}$ and using the particle conservation property one obtains from Eqs. (E.15) and (E.53)

$$\frac{n_a}{\tau_{ab}} T_a \mathsf{M}_{1m'}^{ab,(0)}(\gamma_{ab}) = -\frac{n_b}{\tau_{ba}} T_b \mathsf{N}_{1m'}^{ba,(0)}(\gamma_{ba}). \tag{E.96}$$

Combining Eq. (E.96) with Eq. (E.55) one arrives at the formula

$$\mathsf{M}_{1m'}^{ab,(0)}(\gamma_{ab}) = -\frac{T_a}{T_b} \gamma_{ba} \mathsf{N}_{1m'}^{ba,(0)}(\gamma_{ba}), \tag{E.97}$$

where the matrix elements on the right-hand side of the last equation reads [cf. Eq. (E.68)],

$$\mathsf{N}_{1m'}^{ba,(0)}(\gamma_{ba}) = \frac{3}{\sqrt{\pi}} \frac{\Gamma(m'+1/2)}{m'!} \frac{\gamma_{ba}}{(1+\gamma_{ba}^2)^{m'+3/2}} \times \left[2m'(1+\gamma_{ba}^2) - (2m'+1)\left(1-\frac{T_b}{T_a}\right) \right].$$
(E.98)

Replacing in Eqs. (E.46)-(E.51) for m'=1 and for $\ell=0$, respectively, one obtains

$$\mathsf{M}_{1m'}^{ab,(0)}(\gamma_{ab}) = \frac{3}{2\sqrt{\pi}\gamma_{ab}} \sum_{i=0}^{m'+1} \left[X_{1m'}^{(0),i} \, p_{\nu}^{(0),i}(\gamma_{ab}) - Y_{1m'}^{(0),i} \, p_{D}^{(0),i}(\gamma_{ab}) + \left(1 - \frac{T_a}{T_b}\right) Z_{1m'}^{(0),i} \, p_{D}^{(0),i+1}(\gamma_{ab}) \right], \tag{E.99}$$

with

$$X_{1m'}^{(0),i} = 0,$$
 (E.100)

$$Y_{1m'}^{(0),i} = 2\sum_{j=0}^{i} S_{1m'}^{(0),ji-j} 2j(2i-2j) = \frac{8(-1)^{i}}{(i-2)!} {m'+1/2 \choose m'+1-i}, \text{ (E.101)}$$

$$Z_{1m'}^{(0),i} = 4 \sum_{j=0}^{i} S_{1m'}^{(0),ji-j} 2j = \frac{8(-1)^i}{(i-1)!} {m'+1/2 \choose m'+1-i},$$
 (E.102)

and

$$p_D^{(0),i}(\gamma) = \frac{\Gamma(i+1/2)}{(1+\gamma^2)^{i-1/2}} \left[F(1,i-\frac{1}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) - \frac{F(1,i+\frac{1}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2})}{(1+\gamma^2)} \right]$$

$$= \frac{\Gamma(i-1/2)}{2(1+\gamma^2)^{i-1/2}} \left[F(1,i-\frac{1}{2};\frac{3}{2};\frac{\gamma^2}{1+\gamma^2}) - 1 \right]. \tag{E.103}$$

Inserting Eq. (E.100)-(E.103) into Eq. (E.99) yields

$$\mathsf{M}_{1m'}^{ab,(0)}(\gamma) = -\frac{6}{\sqrt{\pi}\gamma} \sum_{i=0}^{m'+1} \binom{m'+1/2}{m'+1-i} \left\{ \cdot \right\},\tag{E.104}$$

where the brackets represent

$$\left\{ \cdot \right\} = \frac{(-1)^{i}}{(i-2)!} \frac{\Gamma(i-1/2)}{(1+\gamma)^{i-1/2}} \left[F(1, i - \frac{1}{2}; \frac{3}{2}; \frac{\gamma^{2}}{1+\gamma^{2}}) - 1 \right]
- \left(1 - \frac{T_{a}}{T_{b}} \right) \frac{(-1)^{i}}{(i-1)!} \frac{\Gamma(i+1/2)}{(1+\gamma)^{i+1/2}} \left[F(1, i + \frac{1}{2}; \frac{3}{2}; \frac{\gamma^{2}}{1+\gamma^{2}}) - 1 \right] . (E.105)$$

The following relations have been obtained by means of Maple [48]

$$\sum_{i=0}^{m'+1} \frac{(-1)^i}{(i-2)!} {m'+1/2 \choose m'+1-i} \frac{\Gamma(i-1/2)}{(1+\gamma^2)^i} = \frac{\sqrt{\pi}}{2} {m'+1/2 \choose m'-1} \frac{F(1-m', \frac{3}{2}; \frac{5}{2}; \frac{1}{1+\gamma^2})}{(1+\gamma^2)^2}$$
(E.106)

$$\sum_{i=0}^{m'+1} \frac{(-1)^i}{(i-2)!} {m'+1/2 \choose m'+1-i} \frac{\Gamma(i-1/2)}{(1+\gamma^2)^i} F(1, i-\frac{1}{2}; \frac{3}{2}; \frac{\gamma^2}{1+\gamma^2})$$

$$= \frac{\sqrt{\pi}}{2} {m'-1/2 \choose m'-1} \frac{F(1-m', \frac{1}{2}; \frac{3}{2}; \frac{1}{1+\gamma^2})}{(1+\gamma^2)} \quad (E.107)$$

$$\sum_{i=0}^{m+1} \frac{(-1)^{i}}{(i-1)!} {m'+1/2 \choose m'+1-i} \frac{\Gamma(i+1/2)}{(1+\gamma^{2})^{i}}$$

$$= -\frac{\sqrt{\pi}}{2} {m'+1/2 \choose m'} \frac{F(-m', \frac{3}{2}; \frac{3}{2}; \frac{1}{1+\gamma^{2}})}{(1+\gamma^{2})}$$

$$= -\frac{\sqrt{\pi}}{2} {m'+1/2 \choose m'} \frac{\gamma^{2m'}}{(1+\gamma^{2})^{m'+1}}$$
 (E.108)

$$\sum_{i=0}^{m'+1} \frac{(-1)^i}{(i-1)!} {m'+1/2 \choose m'+1-i} \frac{\Gamma(i+1/2)}{(1+\gamma^2)^i} F(1, i+\frac{1}{2}; \frac{3}{2}; \frac{\gamma^2}{1+\gamma^2})$$

$$= -\frac{\sqrt{\pi}}{2} {m'-1/2 \choose m'} F(-m', \frac{1}{2}; \frac{1}{2}; \frac{1}{1+\gamma^2})$$

$$= -\frac{\sqrt{\pi}}{2} {m'-1/2 \choose m'} \frac{\gamma^{2m'}}{(1+\gamma^2)^{m'}}.$$
(E.109)

These equations can be combined to yield

$$\mathsf{M}_{1m'}^{ab,(0)}(\gamma) = -\frac{3}{\gamma(1+\gamma^2)^{1/2}} \left\{ \binom{m'-1/2}{m'-1} F(1-m', \frac{1}{2}; \frac{3}{2}; \frac{1}{1+\gamma^2}) - \binom{m'+1/2}{m'-1} \frac{F(1-m', \frac{3}{2}; \frac{5}{2}; \frac{1}{1+\gamma^2})}{(1+\gamma^2)} + \left(1 - \frac{T_a}{T_b}\right) \right\} \times \left[\binom{m'-1/2}{m'} \frac{\gamma^{2m'}}{(1+\gamma^2)^{m'}} - \binom{m'+1/2}{m'} \frac{\gamma^{2m'}}{(1+\gamma^2)^{m'+1}} \right] \right\}. (E.110)$$

Applying again Eq. (E.90) one obtains

$$\frac{3}{2} \frac{\gamma^2}{(1+\gamma^2)} F(1-m', \frac{3}{2}; \frac{3}{2}; \frac{1}{1+\gamma^2}) = \frac{3}{2} F(1-m', \frac{1}{2}; \frac{3}{2}; \frac{1}{1+\gamma^2}) - \frac{(m'+1/2)}{(1+\gamma^2)} F(1-m', \frac{3}{2}; \frac{5}{2}; \frac{1}{1+\gamma^2}). \quad (E.111)$$

When this equation is substituted into Eq. (E.110) one finally gets the matrix elements related to the second collisional moment of the differential operator, that is,

$$\begin{split} \mathsf{M}_{1m'}^{ab,(0)}(\gamma_{ab}) &= -\frac{3\gamma_{ab}}{(1+\gamma_{ab}^2)^{3/2}} \frac{m'\Gamma(m'+1/2)}{m'!\Gamma(3/2)} F(1-m',\frac{3}{2};\frac{3}{2};\frac{1}{1+\gamma_{ab}^2}) \\ &+ \left(1-\frac{T_a}{T_b}\right) \frac{3\gamma_{ab}^{2m'-1}}{(1+\gamma_{ab}^2)^{m'+3/2}} \frac{\Gamma(m'+1/2)}{m'!\Gamma(3/2)} \left(m'-\frac{\gamma_{ab}^2}{2}\right) \\ &= -\frac{3}{\sqrt{\pi}} \frac{\Gamma(m'+1/2)}{m'!} \frac{\gamma_{ab}^{2m'-1}}{(1+\gamma_{ab}^2)^{m'+3/2}} \\ &\times \left[2m'(1+\gamma_{ab}^2) - \left(1-\frac{T_a}{T_b}\right) \left(2m'-\gamma_{ab}^2\right)\right]. (\text{E}.112) \end{split}$$

The energy conservation of particles can now be verified by replacing γ_{ab} $1/\gamma_{ba}$ in Eq. (E.112), that is

$$-\frac{T_{b}}{T_{a}\gamma_{ba}}\mathsf{M}_{1m'}^{ba,(0)}(\gamma_{ba}) = \frac{3}{\sqrt{\pi}} \frac{\Gamma(m'+1/2)}{m'!} \frac{\gamma_{ba}^{-1}\gamma_{ba}^{1-2m'}\gamma_{ba}^{2m'+3}}{(1+\gamma_{ba}^{2})^{m'+3/2}} \times \left[\frac{2m'T_{b}(1+\gamma_{ba}^{2})}{T_{a}\gamma_{ba}^{2}} - \left(\frac{T_{b}}{T_{a}} - 1\right) \left(2m' - \frac{1}{\gamma_{ba}^{2}}\right) \right]$$

$$= \frac{3}{\sqrt{\pi}} \frac{\Gamma(m'+1/2)}{m'!} \frac{\gamma_{ba}}{(1+\gamma_{ba}^{2})^{m'+3/2}} \times \left[2m'(1+\gamma_{ba}^{2})\frac{T_{b}}{T_{a}} + \left(1 - \frac{T_{b}}{T_{a}}\right) \left(2m'\gamma_{ba}^{2} - 1\right) \right]$$

$$= \frac{3}{\sqrt{\pi}} \frac{\Gamma(m'+1/2)}{m'!} \frac{\gamma_{ba}}{(1+\gamma_{ba}^{2})^{m'+3/2}} \times \left[2m'(1+\gamma_{ba}^{2}) - (2m'+1) \left(1 - \frac{T_{b}}{T_{a}}\right) \right], \quad (E.113)$$

which agrees with Eq. (E.98).

E.5Comparison to results in literature

In this section it is briefly shown how the Braginskii matrix elements presented in this appendix are related to the corresponding results obtained by various authors during the last decades.

A comparison of Braginskii's definition of matrix elements [cf. Eq. (A.1) of Reference 79] with Eqs. (E.15) and (E.53), respectively, yields

$$M_{mm'}^{ab} = v_{ta}^{2} \frac{n_{a}}{\tau_{ab}} \mathsf{M}_{mm'}^{ab,(1)}$$
 (E.114)
 $N_{mm'}^{ab} = v_{ta} v_{tb} \frac{n_{a}}{\tau_{ab}} \mathsf{N}_{mm'}^{ab,(1)}$. (E.115)

$$N_{mm'}^{ab} = v_{ta}v_{tb}\frac{n_a}{\tau_{ab}}N_{mm'}^{ab,(1)}.$$
 (E.115)

The moments of the collision operator were evaluated by introducing the generating function for the Laguerre polynomials which leads to the equations

$$\frac{n_a}{\tau_{ab}} v_{ta}^2 \mathcal{M} = \sum_{m=0}^{\infty} \sum_{m'=0}^{\infty} \xi^m \eta^{m'} M_{mm'}^{ab}$$
 (E.116)

$$\frac{n_a}{\tau_{ab}} v_{ta} v_{tb} \mathcal{N} = \sum_{m=0}^{\infty} \sum_{m'=0}^{\infty} \xi^m \eta^{m'} N_{mm'}^{ab}.$$
 (E.117)

The generating formulas from which the matrix elements were calculated of by Taylor expanding the functions \mathcal{M} and \mathcal{N} around $\xi = 0$ and $\eta = 0$, respectively, read [cf. Eq. (A.4) of Reference 79]

$$\mathcal{M}(\xi, \eta, \gamma_{ab}, T_a, T_b) = -\frac{\gamma_{ab}}{2(1 - \xi \eta)^{3/2} (1 - \xi)(1 - \eta)} \times \sqrt{\frac{1 + x + y}{1 + x + y + \gamma_{ab}^2}} \left\{ \cdot \right\},$$
 (E.118)

with

$$\left\{ \cdot \right\} = 1 - \frac{x+y}{1+x+y+\gamma_{ab}^2} + \frac{5xy}{(1+x+y+\gamma_{ab}^2)^2} + \frac{2xy\gamma_{ab}^2}{(1+x+y)(1+x+y+\gamma_{ab}^2)^2} - \left(1 - \frac{T_a}{T_b}\right) \left[\frac{1}{1+x+y+\gamma_{ab}^2} - \frac{5x}{(1+x+y+\gamma_{ab}^2)^2} - \frac{2x\gamma_{ab}^2}{(1+x+y)(1+x+y+\gamma_{ab}^2)^2}\right], \quad (E.119)$$

as well as

$$\mathcal{N}(\xi, \eta, \gamma_{ab}, T_a, T_b) = \frac{T_a}{2T_b(1-\xi)(1-\eta)} \sqrt{\frac{(1+x)(1+y)}{1+x+\gamma_{ab}^2(1+y)}} \left\{ \cdot \right\}, \quad (\text{E}.120)$$

with

$$\left\{ \cdot \right\} = 1 - \frac{x + \gamma_{ab}^2 y}{1 + x + \gamma_{ab}^2 (1 + y)} + \frac{3xy \gamma_{ab}^2}{[1 + x + \gamma_{ab}^2 (1 + y)]^2} + \left(\frac{T_b}{T_a} - 1 \right) \left[\frac{\gamma_{ab}^2}{1 + x + \gamma_a^2 (1 + y)} - \frac{3x \gamma_{ab}^2}{[1 + x + \gamma_a^2 (1 + y)]^2} \right], \quad (E.121)$$

where $x = \xi/(1-\xi)$ and $y = \eta/(1-\eta)$. The matrix elements computed from these expressions are valid for $\ell = 1$ and for arbitrary species temperatures.

In Reference 80 Hirshman defined the matrix elements by

$$M_{mm'}^{ab} \equiv \frac{\tau_{ab}}{n_a} \int d^3v \frac{v_{\parallel}}{v_{ta}} L_m^{(3/2)}(x^2) \mathcal{C}_{ab} \left[\frac{2v_{\parallel}}{v_{ta}} L_{m'}^{(3/2)}(x^2) f_{a0}, f_{b0} \right]$$
 (E.122)

$$N_{mm'}^{ab} \equiv \frac{\tau_{ab}}{n_a} \int d^3v \frac{v_{\parallel}}{v_{ta}} L_m^{(3/2)}(x^2) \mathcal{C}_{ab} \left[f_{a0}, \frac{2v_{\parallel}}{v_{tb}} L_{m'}^{(3/2)}(y^2) f_{b0} \right], \quad (E.123)$$

and used more or less the same method as Braginskii in evaluating these integrals. The corresponding matrix elements are valid for $\ell = 1$ and for

 $T_a = T_b$. From Eqs. (E.122) and (E.123) as well as Eqs. (E.15) and (E.53) one can conclude that

$$M_{mm'}^{ab} = 2M_{mm'}^{ab,(1)}$$
 (E.124)
 $N_{mm'}^{ab} = 2N_{mm'}^{ab,(1)}$. (E.125)

$$N_{mm'}^{ab} = 2N_{mm'}^{ab,(1)}.$$
 (E.125)

In the paper by Wong [82] the collision matrix elements were defined the same way [see Eqs. (6) and (7) therein] as in this appendix, therefore the following equations hold

$$M_{mm'}^{(\ell)} = \mathsf{M}_{mm'}^{ab,(\ell)}$$
 (E.126)
 $N_{mm'}^{(\ell)} = \mathsf{N}_{mm'}^{ab,(\ell)}$. (E.127)

$$N_{mm'}^{(\ell)} = N_{mm'}^{ab,(\ell)}.$$
 (E.127)

The evaluation of these matrix elements was also based on a generating function technique valid for arbitrary ℓ and for equal species temperatures $T_a = T_b$.

Finally, in the work by Ji and Held [90] the collision matrix elements corresponding to the test and field particle operators [Eqs. (56a) and (56b) in Reference 90 have been obtained by a direct evaluation of moments of the Coulomb operator (that is the product of velocity polynomials and the collision operator has been integrated). The results are valid for arbitrary ℓ as well as for arbitrary species temperatures and are related to the matrix elements calculated in the previous sections via the equations

$$A_{ab}^{lmm'} = (2\ell+1)\mathsf{M}_{mm'}^{ab,(\ell)}$$
 (E.128)

$$A_{ab}^{lmm'} = (2\ell + 1)\mathsf{M}_{mm'}^{ab,(\ell)}$$
 (E.128)
 $B_{ab}^{lmm'} = (2\ell + 1)\mathsf{N}_{mm'}^{ab,(\ell)}$. (E.129)

Appendix F

Toroidally symmetric test configuration

In the axisymmetric limit analytic solutions of the standard neoclassical transport theory are available. In this appendix a simple toroidally symmetric test configuration ('standard tokamak') is constructed which can be used to compare the numerical results obtained by the NEO-2 code with known analytical results [22,37,38,56,59–61,94] and, therefore, serves as a benchmark configuration.

The first two sections in this appendix present a compilation of the relevant formulas which are needed in constructing the standard tokamak and are mainly taken from References 91 and 95, respectively.

F.1 3D magnetic fields with nested surfaces

In 3D equilibrium configurations with nested magnetic surfaces the magnetic field can be written in the contravariant (or Clebsch) representation [91,95]

where

$$\nu(\psi, \theta, \varphi) = \theta - \iota(\psi) \varphi + \lambda(\psi, \theta, \varphi). \tag{F.2}$$

One can show that this is a consequence of $\nabla \cdot \mathbf{B} = 0$ and $\mathbf{B} \cdot \nabla \psi = 0$. Combining the equations $\mathbf{j} \cdot \nabla \psi = 0$ and $\mathbf{j} = (c/4\pi) \nabla \times \mathbf{B}$, the magnetic field in the covariant representation can be expressed as [91,95]

where

$$\eta(\psi, \theta, \varphi) = I(\psi) \theta + J(\psi) \varphi + \omega(\psi, \theta, \varphi), \tag{F.4}$$

and $\beta = \beta(\psi, \theta, \varphi)$. The three functions λ, ω and β are periodic with respect to the poloidal and toroidal angles. Using

$$\nabla \lambda = \lambda_{,\theta} \nabla \psi + \lambda_{,\theta} \nabla \theta + \lambda_{,\varphi} \nabla \varphi \tag{F.5}$$

and

$$\nabla \omega = \omega_{,\psi} \nabla \psi + \omega_{,\theta} \nabla \theta + \omega_{,\omega} \nabla \varphi , \qquad (F.6)$$

where, e.g., $\lambda_{,\psi} \equiv \partial \lambda/\partial \psi$, one finds for the contravariant and covariant representation of **B**, respectively,

$$\mathbf{B} = (1 + \lambda_{\theta}) \nabla \psi \times \nabla \theta + (\iota - \lambda_{\varphi}) \nabla \varphi \times \nabla \psi \tag{F.7}$$

$$= \frac{(1+\lambda_{,\theta})}{\sqrt{g}}\mathbf{e}_{\varphi} + \frac{(t-\lambda_{,\varphi})}{\sqrt{g}}\mathbf{e}_{\theta}$$
 (F.8)

$$\equiv B^{\varphi} \mathbf{e}_{\varphi} + B^{\theta} \mathbf{e}_{\theta}, \tag{F.9}$$

and

$$\mathbf{B} = (I + \omega_{,\theta})\nabla\theta + (J + \omega_{,\varphi})\nabla\varphi + (\beta + \theta I_{,\psi} + \varphi J_{,\psi} + \omega_{,\psi})\nabla\psi \text{ (F.10)}$$

$$\equiv B_{\theta}\nabla\theta + B_{\varphi}\nabla\varphi + B_{\psi}\nabla\psi. \tag{F.11}$$

The Jacobian of the (ψ, θ, φ) coordinate system can be found by dotting together the contravariant and covariant representation of **B** yielding

$$\sqrt{g} \equiv \frac{1}{\nabla \psi \cdot \nabla \theta \times \nabla \varphi}$$

$$= \frac{1}{B^2} \left[(\iota - \lambda_{,\varphi}) \left(I + \omega_{,\theta} \right) + (1 + \lambda_{,\theta}) \left(J + \omega_{,\varphi} \right) \right].$$
(F.12)

The single-valued function $\lambda(\psi, \theta, \varphi)$ can be determined from the condition that the current density **j** lies in the flux surface,

$$\mathbf{j} \cdot \nabla \psi = 0 \,, \tag{F.13}$$

which is equivalent to

$$\frac{\partial B_{\varphi}}{\partial \theta} - \frac{\partial B_{\theta}}{\partial \varphi} = 0. \tag{F.14}$$

From Ampère's law, $\mathbf{j} = (c/4\pi) \nabla \times \mathbf{B}$, it can be shown that the quantities I and J are proportional to the total toroidal and poloidal current. The total toroidal current inside a flux surface is cI/2 and the total poloidal current outside a flux surface is cJ/2, where I and J are calculated from

$$I(\psi) = \frac{1}{2\pi} \int_{0}^{2\pi} d\theta B_{\theta}$$
 (F.15)

$$J(\psi) = \frac{1}{2\pi} \int_{0}^{2\pi} d\varphi B_{\varphi}. \tag{F.16}$$

F.2 Transformation to Boozer coordinates

Magnetic coordinates with the property that the covariant components of the magnetic field, B_{θ} and B_{φ} , respectively, represent flux functions are called Boozer coordinates [22,96]. The stream functions ν and η have the form

$$\nu(\psi, \theta_B, \varphi_B) = \theta_B - \iota(\psi)\varphi_B \tag{F.17}$$

$$\eta(\psi, \theta_B, \varphi_B) = I(\psi)\theta_B + J(\psi)\varphi_B.$$
(F.18)

The transformation from general flux coordinates (ψ, θ, φ) to Boozer coordinates $(\psi, \theta_B, \varphi_B)$ is defined by [95]

$$\theta_B = \theta + \tilde{\theta}(\theta, \varphi)$$
 (F.19)

$$\varphi_B = \varphi + \tilde{\varphi}(\theta, \varphi) , \qquad (F.20)$$

where the periodic functions $\tilde{\theta}$ and $\tilde{\varphi}$ are computed from the solution of the relations

$$\theta_B - \iota \varphi_B = \theta - \iota \varphi + \lambda(\theta, \varphi)$$
 (F.21)

$$I \theta_B + J \varphi_B = I \theta + J \varphi + \omega(\theta, \varphi).$$
 (F.22)

Upon substituting Eqs. (F.19) and (F.20) into Eqs. (F.21) and (F.22), one finds

$$\tilde{\theta}(\theta,\varphi) = \frac{\iota \omega + J \lambda}{J + \iota I}$$
 (F.23)

$$\tilde{\varphi}(\theta, \varphi) = \frac{\omega - I \lambda}{J + \iota I}.$$
(F.24)

F.3 Tokamak with circular cross section

F.3.1 Construction of an "equilibrium"

By definition, in the toroidally symmetric test configuration the magnetic surfaces are nested concentric circular tori with constant major radius R_0 . The best adapted coordinate system in this geometry is the toroidal coordinate system (r, θ, φ) defined by

$$R(r,\theta) = R_0 + r\cos\theta \tag{F.25}$$

$$Z(r,\theta) = r \sin \theta$$
 (F.26)

$$\phi = \varphi , \qquad (F.27)$$

where r is the minor radius and θ and φ are the geometrical poloidal and toroidal angles, respectively¹. Further prescribed quantities are the rotational transform ι and the toroidal flux at the last closed magnetic surface, ψ' . If one replaces the geometrical radius r by $a\sqrt{s}$, where a is the radius of the outermost flux surface and $s = \psi(s)/\psi(1)$ is the normalized toroidal flux, one obtains the quasi-toroidal coordinates (ψ, θ, φ) . The quantity ψ (or s, respectively) can be interpreted as a topological radius. Since the quasi-toroidal coordinate system is an orthogonal one the off-diagonal metric coefficients are all zero. The Jacobian of these coordinates and the covariant metric coefficients are

$$\sqrt{g} \equiv \frac{\partial(x, y, z)}{\partial(\psi, \theta, \varphi)} = \frac{a^2 R}{2\psi'} = \frac{R_0}{\mathscr{B}_0} \hat{R} , \qquad (F.28)$$

as well as

$$g_{\psi\psi} = \frac{a^2}{4s\psi'^2} = \frac{1}{\epsilon^2 \mathcal{B}_0^2 R_0^2}$$
 (F.29)

$$g_{\theta\theta} = a^2 s = \epsilon^2 R_0^2 \tag{F.30}$$

$$g_{\varphi\varphi} = R_0^2 \hat{R}^2, \tag{F.31}$$

where the abbreviations $\mathscr{B}_0 \equiv 2\psi'/a^2$, $\epsilon \equiv r/R_0$ and $\hat{R} \equiv R/R_0 = 1 + \epsilon \cos \theta$ have been introduced.

Using the expressions from the previous sections and taking into account the axisymmetry, $\partial/\partial\varphi = 0$, the contravariant components of **B** become [see Eqs. (F.8) and (F.9)]

$$B^{\varphi} = \frac{(1+\lambda_{,\theta})}{\sqrt{g}} , \quad B^{\theta} = \frac{\iota}{\sqrt{g}}.$$
 (F.32)

One can change the contravariant components into covariant components with $B_i = g_{ij} B^j$, leading to

$$B_{\theta} = g_{\theta\theta} B^{\theta} = \epsilon^2 \iota \mathcal{B}_0 R_0 \hat{R}^{-1}$$
 (F.33)

$$B_{\varphi} = g_{\varphi\varphi} B^{\varphi} = \mathscr{B}_0 R_0 \hat{R} (1 + \lambda_{\theta}). \tag{F.34}$$

In axisymmetric systems, Eq. (F.14) reduces to the fact that B_{φ} is a flux surface quantity which, in turn, requires $\hat{R}(1 + \lambda_{,\theta})$ being independent of θ . Hence,

$$f(\psi) = \hat{R}(1 + \lambda_{\theta}) \tag{F.35}$$

¹Of course, full vacuum equation, $\nabla \times \mathbf{B} = 0$, cannot be satisfied if Eqs. (F.25)-(F.27) are assumed. Some additional currents on the flux surfaces are needed. However, if the configuration is such that the inverse aspect ratio $\bar{\epsilon} \equiv a/R_0 \ll 1$ the proposed magnetic field model should be a useful approximation to a realistic MHD equilibrium [97].

and

$$\lambda_{,\theta} = \frac{f(\psi)}{\hat{R}} - 1. \tag{F.36}$$

The integral with respect to θ of the function $\lambda_{,\theta}$ vanishes because λ is periodic in θ , that is

$$\int_{0}^{2\pi} d\theta \lambda_{,\theta} = \lambda(\psi, 2\pi) - \lambda(\psi, 0) = 0 = f(\psi) \int_{0}^{2\pi} \frac{d\theta}{\hat{R}} - 2\pi , \qquad (F.37)$$

from which it follows that

$$f(\psi) = \left(\frac{1}{2\pi} \int_{0}^{2\pi} \frac{\mathrm{d}\theta}{\hat{R}(\psi, \theta)}\right)^{-1} \equiv \langle \hat{R}^{-1} \rangle^{-1} , \qquad (F.38)$$

and the stream function λ is finally given by

$$\lambda(\psi, \theta) = \frac{1}{\langle \hat{R}^{-1} \rangle} \int_{0}^{\theta} \frac{\mathrm{d}\theta'}{\hat{R}(\psi, \theta')} - \theta . \tag{F.39}$$

Here, Eq. (F.36) can be rewritten as

$$1 + \lambda_{,\theta} = \frac{1}{\langle \hat{R}^{-1} \rangle \, \hat{R}} \,, \tag{F.40}$$

and the co- and contravariant components of the magnetic field then have the form

$$B^{\varphi} = \frac{\mathscr{B}_0}{\langle \hat{R}^{-1} \rangle R_0 \hat{R}^2} = \frac{J}{R_0^2 \hat{R}^2}$$
 (F.41)

$$B^{\theta} = \frac{t\mathscr{B}_0}{R_0\hat{R}} = \frac{tJ\langle\hat{R}^{-1}\rangle}{R_0^2\hat{R}}$$
 (F.42)

$$B_{\varphi} = \frac{\mathscr{B}_0 R_0}{\langle \hat{R}^{-1} \rangle} = J \tag{F.43}$$

$$B_{\theta} = \epsilon^2 \iota \mathcal{B}_0 R_0 \hat{R}^{-1} = \frac{I}{\langle \hat{R}^{-1} \rangle \hat{R}}, \qquad (F.44)$$

where the poloidal and toroidal currents in quasi-toroidal coordinates have been calculated by means of Eqs. (F.15) and (F.16), respectively,

$$J(\psi) = \frac{1}{2\pi} \int_{0}^{2\pi} d\varphi B_{\varphi} = B_{\varphi} = \frac{\mathscr{B}_{0} R_{0}}{\langle \hat{R}^{-1} \rangle}$$
 (F.45)

$$I(\psi) = \frac{1}{2\pi} \int_{0}^{2\pi} d\theta B_{\theta} = \epsilon^{2} \iota \mathcal{B}_{0} R_{0} \langle \hat{R}^{-1} \rangle = \epsilon^{2} \iota J \langle \hat{R}^{-1} \rangle^{2}. \quad (F.46)$$

Hence, it follows that the square of the magnetic field strength can be represented by

$$B^{2} = B^{\theta} B_{\theta} + B^{\varphi} B_{\varphi} = \frac{iJ \langle \hat{R}^{-1} \rangle}{R_{0}^{2} \hat{R}} \frac{I}{\langle \hat{R}^{-1} \rangle \hat{R}} + \frac{J}{R_{0}^{2} \hat{R}^{2}} J,$$
 (F.47)

where Eqs. (F.41)-(F.46) have been applied. Finally, one obtains for the magnetic field strength in quasi-toroidal coordinates the relation

$$B(\psi, \theta) = \frac{\sqrt{J(J + tI)}}{R_0 \hat{R}}.$$
 (F.48)

F.3.2 Transformation to Boozer coordinates

From Eqs. (F.10), (F.11) and (F.44) one obtains

$$\omega_{,\theta} = B_{\theta} - I = \frac{I}{\langle \hat{R}^{-1} \rangle \hat{R}} - I. \tag{F.49}$$

Integration with respect to θ yields

$$\omega(\psi,\theta) = I\left(\frac{1}{\langle \hat{R}^{-1} \rangle} \int_{0}^{\theta} \frac{\mathrm{d}\theta'}{\hat{R}(\psi,\theta')} - \theta\right) = I(\psi)\lambda(\psi,\theta) , \qquad (F.50)$$

from which it follows that Eqs. (F.23) and (F.24) reduce to

$$\tilde{\varphi} = \frac{\omega - I \lambda}{J + t I} = \frac{I \lambda - I \lambda}{J + t I} = 0$$
 (F.51)

$$\tilde{\theta} = \frac{\iota \omega + J \lambda}{J + \iota I} = \frac{\iota I \lambda + J \lambda}{J + \iota I} = \lambda.$$
 (F.52)

Therefore, on surfaces of constant toroidal flux ψ the quasi-toroidal coordinate system is related to the Boozer coordinate system through

$$\theta_B(\theta) = \theta + \lambda(\theta)$$
 (F.53)

$$\varphi_B = \varphi , \qquad (F.54)$$

or, more explicitly,

$$\theta_B = \frac{1}{\langle \hat{R}^{-1} \rangle} \int_0^{\theta} \frac{\mathrm{d}\theta'}{\hat{R}(\theta')} , \qquad (F.55)$$

where Eq. (F.39) has been used. The integral appearing in Eq. (F.55) can be evaluated to obtain

$$\int_{0}^{\theta} \frac{d\theta'}{\hat{R}(\theta')} = \frac{2}{\sqrt{1 - \epsilon^2}} \arctan\left\{\frac{(1 - \epsilon)\tan(\theta/2)}{\sqrt{1 - \epsilon^2}}\right\}, \quad (F.56)$$

and the quantity $\langle \hat{R}^{-1} \rangle$ is

$$\langle \hat{R}^{-1} \rangle = \frac{1}{2\pi} \int_{0}^{2\pi} \frac{\mathrm{d}\theta}{1 + \epsilon \cos \theta} = \frac{1}{\sqrt{1 - \epsilon^2}}, \quad \text{for } \epsilon^2 < 1.$$
 (F.57)

The final step consists in calculating the Boozer spectra of R, Z and B. This could be achieved by inverting Eq. (F.55) to get

$$\theta(\theta_B) = 2 \arctan \left\{ \frac{\sqrt{1 - \epsilon^2} \tan(\theta_B/2)}{(1 - \epsilon)} \right\} ,$$
 (F.58)

and, upon using the relation

$$\tan\frac{\alpha}{2} = \sqrt{\frac{1 - \cos\alpha}{1 + \cos\alpha}},\tag{F.59}$$

one obtains the following expressions.

$$\cos \theta = \frac{\cos \theta_B - \epsilon}{1 - \epsilon \cos \theta_B} \tag{F.60}$$

$$\sin \theta = \frac{\sqrt{1 - \epsilon^2} \sin \theta_B}{1 - \epsilon \cos \theta_B}.$$
 (F.61)

Therefore, the representation for R, Z and B [see Eqs. (F.25), (F.26) and (F.48)] in Boozer coordinates is given by

$$\hat{R}(\theta_B) \equiv \frac{R}{R_0} = \frac{1 - \epsilon^2}{1 - \epsilon \cos \theta_B}$$
 (F.62)

$$\hat{Z}(\theta_B) \equiv \frac{Z}{R_0} = \frac{\epsilon\sqrt{1-\epsilon^2}\sin\theta_B}{1-\epsilon\cos\theta_B}$$
 (F.63)

$$B(\theta_B) = \frac{\sqrt{J(J+\iota I)}}{R_0} \frac{(1-\epsilon\cos\theta_B)}{(1-\epsilon^2)}.$$
 (F.64)

The Fourier expansion for R, Z and B has the following form

$$R(\theta_B) = \sum r_m \cos \theta_B \tag{F.65}$$

$$Z(\theta_B) = \sum_{m} z_m \sin \theta_B \tag{F.66}$$

$$B(\theta_B) = \sum_m b_m \cos \theta_B, \qquad (F.67)$$

with the Fourier coefficients

$$r_0 = \frac{R_0}{\pi} \int_0^{\pi} d\theta_B \hat{R}(\theta_B)$$
 (F.68)

$$r_m = \frac{2R_0}{\pi} \int_0^{\pi} d\theta_B \hat{R}(\theta_B) \cos(m\theta_B), \quad \text{for } m \ge 1$$
 (F.69)

$$z_0 = 0 (F.70)$$

$$z_m = \frac{2R_0}{\pi} \int_0^{\pi} d\theta_B \hat{Z}(\theta_B) \sin(m\theta_B), \quad \text{for } m \ge 1. \quad (F.71)$$

These coefficients may be calculated by using [29]

$$\int_0^{\pi} dx \frac{\cos(nx)}{1 + a\cos x} = \frac{\pi}{\sqrt{1 - a^2}} \left(\frac{\sqrt{1 - a^2} - 1}{a}\right)^n, \quad \text{for } a^2 < 1, \quad (F.72)$$

as well as

$$\int_0^{\pi} dx \frac{\sin x \sin(nx)}{(1 - 2a\cos x + a^2)} = \frac{\pi}{2} a^{n-1} , \quad \text{for} \quad a^2 < 1, \quad n \ge 1. \quad (F.73)$$

Hence, it follows that

$$r_{0} = \frac{R_{0}(1 - \epsilon^{2})}{\pi} \frac{\pi}{\sqrt{1 - \epsilon^{2}}} = R_{0}\sqrt{1 - \epsilon^{2}}$$

$$r_{m} = \frac{2R_{0}(1 - \epsilon^{2})}{\pi} \frac{\pi}{\sqrt{1 - \epsilon^{2}}} \left(\frac{1 - \sqrt{1 - \epsilon^{2}}}{\epsilon}\right)^{m}$$

$$= 2R_{0}\sqrt{1 - \epsilon^{2}} \left(\frac{1 - \sqrt{1 - \epsilon^{2}}}{\epsilon}\right)^{m} , \quad \text{for } m \ge 1$$

$$z_{m} = \frac{2R_{0}}{\pi} \epsilon \sqrt{1 - \epsilon^{2}} \frac{\pi}{2} \frac{2}{\epsilon} \left(\frac{1 - \sqrt{1 - \epsilon^{2}}}{\epsilon}\right)^{m}$$

$$= 2R_{0}\sqrt{1 - \epsilon^{2}} \left(\frac{1 - \sqrt{1 - \epsilon^{2}}}{\epsilon}\right)^{m}$$

$$= r_{m}, \quad \text{for } m \ge 1.$$

$$(F.76)$$

The Fourier coefficients for B can be immediately obtained from Eq. (F.64) leading to

$$b_0 = \frac{\sqrt{J(J+\iota I)}}{R_0(1-\epsilon^2)}$$

$$= \mathscr{B}_0 \frac{\sqrt{1 - \epsilon^2 + \epsilon^2 t^2}}{1 - \epsilon^2} \tag{F.77}$$

$$b_1 = -\epsilon b_0. (F.78)$$

F.4 Comparison with the standard model

A widely used magnetic field model in the literature is the so-called standard model defined in the toroidal coordinate system (r, θ, φ) by (for details see Reference 56)

$$\mathbf{B}(r,\theta) = B_0 \,\epsilon(r) \,\epsilon(r) \,\hat{\mathbf{e}}_{\theta} + \frac{B_0}{1 + \epsilon(r)\cos\theta} \,\hat{\mathbf{e}}_{\varphi} \,\,, \tag{F.79}$$

where B_0 is a constant having the dimension of a magnetic field and $\hat{\mathbf{e}}_i$ are the physical basis vectors. It has to be noted that this model field is not divergence-free². Using the relation $\psi = \mathcal{B}_0 r^2/2$ between the toroidal flux ψ and the minor radius r the magnetic field model calculated in Section (F.3.1) can be expressed as

$$\mathbf{B}(r,\theta) = \frac{\mathscr{B}_0}{1 + \epsilon(r)\cos\theta} \left[\iota(r)\epsilon(r)\,\hat{\mathbf{e}}_{\theta} + \sqrt{1 - \epsilon(r)^2}\,\hat{\mathbf{e}}_{\varphi} \right]. \tag{F.80}$$

Using $\mathscr{B}_0 \equiv B_0$ the standard model is obtained from Eq. (F.80) by neglecting terms of $\mathcal{O}(\epsilon^2)$.

²more precisely, $(r/B_0)\nabla \cdot \mathbf{B} \sim \mathcal{O}(\epsilon^2)$

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