

TOPICS IN LABORATORY PLASMA INSTABILITY AND TURBULENCE



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To my family

ABSTRACT

The first part of this thesis investigates the growth of ion density perturbations in large-amplitude laser-driven wakefields via two-dimensional particle-in-cell simulations. Growth rates and wave numbers of the perturbations are found to be consistent with a longitudinal strong-field modulational instability. We examine the transverse dependence of the instability for a Gaussian wakefield envelope and show that growth rates and wavenumbers can be maximised off-axis. On-axis growth rates are found to decrease with increasing ion mass or electron temperature. These results are in close agreement with theoretical predictions obtained by solving the dispersion relation for a long-wavelength electrostatic oscillation in resonance with the plasma frequency and energy density that is large compared to the plasma thermal energy density. The implications for wakefield accelerators – in particular multi-pulse schemes – and methods to mitigate the effects of ion dynamics are discussed.

In the second part of the thesis, we develop a linearised Fokker-Planck collision model for gyrokinetic simulations that satisfies conservation laws and is accurate at arbitrary collisionality. The differential test-particle component of the operator is exact; the implementation of the integrodifferential field-particle component uses a spherical harmonic expansion and a modified Laguerre polynomial expansion introduced by Hirshman and Sigmar [S. P. Hirshman, D. J. Sigmar, *Phys. Fluids* **19**, 1532 (1976)]. The numerical methods of the implementation in the δf -gyrokinetic code `stella` [M. Barnes, F. I. Parra, M. Landreman, *Journal of Comp. Phys.* 391, 365-380 (2019)] are discussed, and conservation properties of the operator are verified. The accuracy of the collision model is demonstrated by computing transport coefficients for the classical Spitzer problem and by performing benchmarks against the collision model of the gyrokinetic solver `GS2`.

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CHAPTER 1

MOTIVATION AND OUTLINE

Understanding the behaviour of plasmas and applying that understanding to control the physical world around us is one of the intellectual and technological frontiers of the present century. Indeed, the development of plasma physics has very closely followed, and in other cases, motivated technological advancements, so that experiment and theory are frequently complementary in plasma physics – not unlike the development of thermodynamics went hand in hand with the rise of steam engines. Plasma is abundant in the universe and is inevitably encountered at high energies when matter dissociates into charged ions and electrons. The resulting state of matter is characterised by high electrical conductivity, and, consequently, collective motion of particles in response to electromagnetic fields. Figure 1.1 shows two instances of plasma particles streaming along a magnetic field, in the solar corona and the Wendelstein 7-X experimental fusion reactor – both evoke the highly energetic, dynamic nature of plasma. Predicting the dynamics of plasma is difficult due to the complex interaction of particles, currents, and fields, giving rise to a wide variety of instabilities and turbulence. In some cases, simplifications can be made to enable theoretical insight, but computational modeling is frequently required. This thesis describes work done by the author on two topics in theoretical and computational plasma physics and is accordingly structured

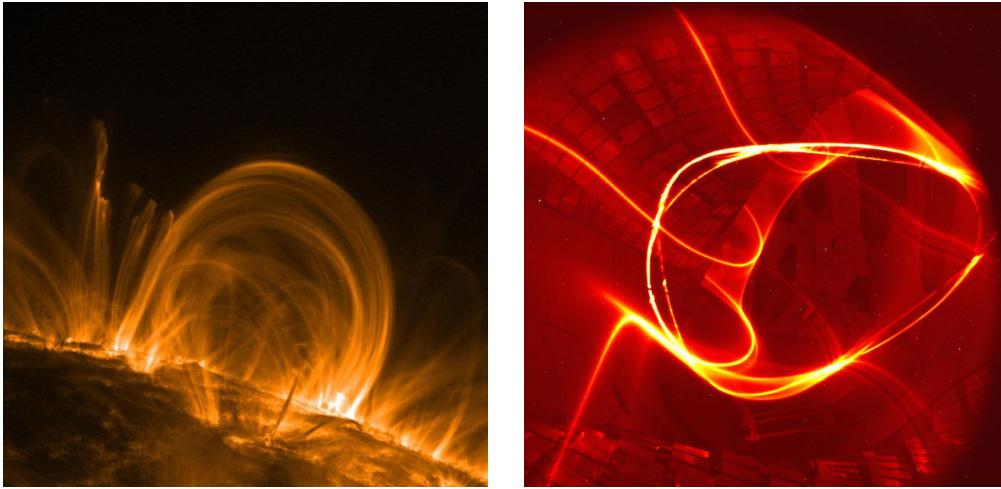


Figure 1.1: *Left:* Plasma streaming along magnetic field lines in the solar corona, imaged by the TRACE satellite. The coronal loops measure up to 30 Earth diameters across. [TRACE, NASA]. *Right:* Trace of electrons streaming along magnetic field lines in the Wendelstein 7-X stellarator, due to partially ionised neutral gas [Max-Planck-Institute for Plasma Physics, Matthias Otte].

in two parts. The current Chapter 1 motivates the work presented here and introduces key concepts. Broadly, Chapters 2 – 5 deal with ion dynamics in laser wakefields. Chapter 3 is an experimental excursion – it describes experiments performed in the Oxford laser-plasma accelerator group to which the author contributed, and presents a design and fluid dynamic modelling of a target for these experiments. Chapter 4 reviews the theory of the modulational instability in a plasma. In Chapter 5, Debye-scale resolution particle-in-cell simulations are performed that show that high-amplitude, linear Langmuir waves in laser-wakefield accelerators drive an unstable growth of ion density perturbations. A detailed comparison of computational results with the theory of high-amplitude electrostatic oscillations in a plasma is performed. Wave numbers, growth rates, and their scalings with ion mass, electron temperature, and wakefield amplitude are shown to be consistent with a longitudinal modulational instability in the strong-field regime. The implications of these

findings for laser wakefield accelerators, and in particular multi-pulse devices, are discussed.

The second part of the thesis, consisting of Chapters 6 – 10, presents a novel Fokker-Planck collision model and its implementation in the gyrokinetic solver **stella** for collisional simulations of turbulence in magnetic confinement fusion reactors of the stellarator type. Chapter 6 introduces nuclear fusion, stellarators, and the gyrokinetic framework. Chapter 7 introduces the Landau-Fokker-Planck collision operator and its salient properties and covers the theory of the proposed collision model. This collision model extends simple approximate operators commonly employed in gyrokinetic simulations to allow for a systematic improvement of the model accuracy. The numerical implementation of the collision model in the gyrokinetic code **stella** is discussed in Chapter 8. Numerical tests of conservation properties, entropy production, and benchmarks against the collision model of the gyrokinetic code **GS2** are provided in Chapter 9. The classical Spitzer problem is solved to demonstrate the flexibility and superior accuracy of the collision model. A summary and outlook on future work are provided in Chapter 10.

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- A. Picksley, A. Alejo, R. J. Shalloo, C. Arran, **A. von Boetticher**, L. Corner, J. A. Holloway, J. Jonnerby, O. Jakobsson, C. Thornton, R. Walczak, and S. M. Hooker (2020), **Meter-Scale, Conditioned Hydrodynamic Optical-Field-Ionized Plasma Channels**, *Physical Review E*, 102, 053201.
- R. J. Shalloo, C. Arran, A. Picksley, **A. von Boetticher**, L. Corner, J. Holloway, G. Hine, J. Jonnerby, H. M. Milchberg, C. Thornton, R. Walczak, S. M. Hooker (2019), **Low-density hydrodynamic optical-field-ionized plasma channels generated with an axicon lens**, *Phys. Rev. Accel. Beams*, 22, 041302.
- **A. von Boetticher**, A. H. M. J. Triaud, D. Queloz et al (2019), **The EBLM Project V. Physical properties of ten fully convective, very-low-mass stars**, *Astronomy and Astrophysics*, 625, A150.
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PART I

MODULATIONAL INSTABILITY IN LASER WAKEFIELDS

CHAPTER 2

INTRODUCTION

2.1 PARTICLE ACCELERATORS

Particle accelerators are an essential tool in physics. They were used to perform the first splitting of the atomic nucleus (Cockroft and Walton, 1932) – confirming the equivalence of mass and energy –, were instrumental in the experimental confirmation of antiparticles (Chamberlain et al., 1955) and the violation of CP symmetry (Christenson et al., 1964), and led to the discovery of the Higgs boson (Aad et al., 2012), to name just some examples. Beyond fundamental physics, they are indispensable as diagnostic tools in experimental science in general, for instance, in the form of Rutherford back-scattering or proton-induced X-ray emission. In thermonuclear fusion research, neutral particle beams from accelerators are used to heat magnetically confined plasma (Speth, 1989). Outside of scientific research, particle beams from accelerators are ubiquitous in medicine – where they are, for instance, used in radiotherapy to treat malignant tumors (e.g. Wilson, 1946; Amaldi, 1999; Levin et al., 2005) and in the generation of X-rays. Indeed, over 60% of accelerators worldwide are employed in industry, with versatile applications including in the manufacture of semiconductors and microchips, for particle beam welding and in

material inspection (Chernyaev and Varzar, 2014). In short, particle accelerators are a structural technology that underpins advancement in a broad set of fields.

Current accelerators are relatively large and expensive devices, ranging from room-sized machines to the 27-km circumference Large Hadron Collider (LHC, Evans and Bryant, 2008) at CERN. The size of an accelerator is roughly set by the required particle beam energy and the available accelerating field strength. To increase the particle energy, one may increase the length of the accelerating stage or the accelerating field strength. Conversely, to obtain compact accelerators without lowering the particle energy, very strong accelerating fields are required. Long accelerating stages can be circularised to make them more compact, as is done in synchrotrons such as the LHC, but the degree of curvature is limited by the attainable field strength of the magnets required to direct the charged particles on a circular path (Evans and Bryant, 2008). On the other hand, the attainable accelerating field strength is limited by material properties since very high potential differences must be controlled for strong electric fields. A solution to these limits is offered by plasma-based particle accelerators.

2.2 PLASMA-BASED ACCELERATORS

Plasma-based particle acceleration (Veksler, 1956; Faĭnberg, 1968) is capable of generating particle beams with energies comparable to those of conventional large-scale accelerators over substantially shorter accelerating distances. This is possible because electrostatic oscillations in a plasma can support electric fields far stronger than those generated in radio-frequency (RF) cavities typically employed in conventional accelerators. A field strength of $\sim 5.5 \text{ MVm}^{-1}$ is realised in the RF acceleration system of the LHC (Evans and Bryant, 2008). In plasma-based accelerators, the maximum attainable field strength is given

by the wave breaking limit: when the oscillation distance of an individual electron exceeds the wavelength of the electrostatic oscillation, phase mixing destroys the coherence of the oscillation (Dawson, 1959). This wave breaking limit is given by $E_{wb} = mc\omega_{pe}/e = m_e c(e^2 n_e / m_e \epsilon_0)^{1/2} / e = (m_e c^2 n_e / \epsilon_0)^{1/2}$ (Tajima and Dawson, 1979). For a plasma density on the order of $n_e \sim 10^{18} \text{ m}^{-3}$, typical in plasma accelerators, this corresponds to a field strength of $\approx 100 \text{ GVm}^{-1}$, thus exceeding typical RF field strengths by four orders of magnitude. As a result, very short accelerating stages can be employed in plasma-based accelerators without conceding beam energy.

The accelerating electric field in plasma-based accelerators is generated by high-frequency oscillations of the electron plasma density. These oscillations can be excited by using a charged particle bunch or laser pulse to displace electrons so that the Coulomb force of the positively charged ion background acts as a restoring force to set up an oscillation of the electron density. In the case of a laser pulse, the mechanism of wave excitation can be understood by considering the oscillations of plasma electrons and ions in the laser field: Since the laser intensity is non-uniform for a finite pulse, the particles experience greater displacements from their equilibrium position in regions of high laser intensity, compared to regions of low laser intensity. This leads to a drift of particles away from regions of high intensity, that is slow compared to the laser frequency. The associated force, known as the ponderomotive force, is given, in the non-relativistic limit, by

$$\mathbf{F}_{\text{pond}} = -\frac{q^2}{16\pi^2 m \omega^2} \nabla E^2 \quad (2.1)$$

where E and ω denote the laser electric field strength and frequency, respectively, and relativistic effects are neglected. Since $E^2 \sim I$, where I denotes the laser intensity, the ponderomotive force can also be interpreted as a force due to a gradient in the radiation pressure. Equation (2.1) implies that the

ponderomotive force does not depend on the polarity of the particles; that is, both electrons and ions are displaced from regions of high laser intensity. However, the heavy ions experience an acceleration that is smaller by a factor $(m_e/m_i)^2$. As a result, electrons are rapidly displaced by the laser pulse and leave behind a region of positive charge. The resulting electric field acts as a restoring force on the electrons, causing them to oscillate at their characteristic plasma frequency.

In this way, a laser propagating through a plasma excites a Langmuir wave (Tonks and Langmuir, 1929) in its wake that has a phase velocity set by the near-luminal speed of the driving pulse. Electrons injected into an accelerating region of this wakefield can be accelerated to relativistic velocities until they dephase with the accelerating structure. Plasma-based accelerators that employ a laser for wakefield excitation are known as laser-wakefield accelerators (LWFA, Tajima and Dawson, 1979). Such devices have been used to generate gigaelectronvolt electron beams over an accelerating distance of only a few centimetres (Leemans et al., 2006; Mangles et al., 2004; Leemans et al., 2014). Applications of wakefield accelerators include, for instance, the generation of ultra-fast hard X-rays (Kneip et al., 2010) and gamma rays (Cipiccia et al., 2011; Ta Phuoc et al., 2012) via betatron emission, and as high-energy electron sources for free-electron lasers (FEL) (Wang et al., 2021). Such light sources enable imaging of processes on extremely short time- and length-scales, including molecular and atomic phenomena (eg. Siders et al., 1999; Rose-Petruck et al., 1999).

A number of variations on the laser wakefield accelerator have been developed, including the plasma wakefield accelerator that drives the electron wave with a charged particle beam, the beat-wave accelerator (Rosenbluth and Liu, 1972; Tajima and Dawson, 1979), the self-modulated wakefield accelerator

(Andreev et al., 1994) and the multi-pulse laser-wakefield accelerator (Umstadter et al., 1994). The beat-wave accelerator introduced the interaction of multiple successive laser pulses with a plasma and alleviated energy requirements for single pulse schemes at a time when chirped-pulse-amplification of laser pulses (CPA, Strickland and Mourou, 1985) was not yet available. The pulse-trains in the beat-wave scheme are generated by the interference of two laser beams of different frequencies ω_1 and ω_2 . If the resulting beat frequency matches the plasma frequency $\Delta\omega = \omega_1 - \omega_2 \approx \omega_{pe}$, a high-amplitude plasma wave is excited resonantly. The multi-pulse accelerator generalizes this concept to a train of laser pulses with a pulse spacing that can, in principle, be arbitrarily varied within a pulse train. While the potential of laser wakefield accelerators has unambiguously been demonstrated, they so far rely on large, high-intensity ($\sim 10^{18} \text{ Wcm}^{-2}$) chirped-pulse-amplification laser systems that are relatively inefficient and cannot operate at high repetition rates that are required for high-flux applications (Hooker et al., 2014).

2.3 MULTI-PULSE WAKEFIELD ACCELERATORS

The repetition rate of present laser-wakefield accelerators, typically on the order of 1 Hz, is too low by orders of magnitude for many applications, such as high-flux light sources or imaging of ultrafast processes using betatron X-ray sources. The excitation of Langmuir waves using trains of successive laser pulses that are resonant with the plasma frequency reduces the laser energy required to drive laser wakefield accelerators. This opens the technology to compact, lower energy lasers capable of operating at the kHz repetition rates required for high-flux light sources and accelerators (Hooker et al., 2014; Cowley et al., 2017). A further advantage of the multi-pulse scheme is the ability for fine control of the plasma wave properties, demonstrated by the targeted

dampening of laser wakefields using a trailing out-of-resonance pulse by Cowley et al. (2017). Compared to the beat-wave accelerator, the multi-pulse approach has the advantage of permitting non-constant spacing between individual pulses in a pulse train. In beat-wave accelerators the inter-pulse spacing is constant, since $\Delta\omega = \omega_1 - \omega_2$. As the wakefield amplitude grows, the relativistic mass increase of electrons leads to an increase in the wakefield wavelength. The resulting mismatch between wakefield wavelength and pulse spacing destroys the resonance between the driving pulse train and the wakefield, thus limiting the wakefield growth (Rosenbluth and Liu, 1972). In multi-pulse accelerators, the inter-pulse spacing can be adjusted to match the relativistic wavelength shift, thus avoiding the Rosenbluth-Liu limit (Umstadter et al., 1994). The pulse-trains required for multi-pulse accelerators can be generated in different ways; methods include the use of arrays of birefringent crystals (Dromey et al., 2007), spectral filtering of a linearly chirped short pulse using a Michelson interferometer (Shalloo et al., 2016) or, elegantly, co-propagating a long, picosecond-duration laser pulse with a low-amplitude plasma wave excited by a seed pulse, with subsequent compression by a dispersive optic (Jakobsson et al., 2021).

CHAPTER 3

LASER WAKEFIELD EXPERIMENTS

3.1 EXPERIMENTAL CAMPAIGNS IN THE OXFORD LASER-PLASMA ACCELERATOR GROUP

3.1.1 PLASMA WAVE-GUIDE EXPERIMENTS

To attain electron beams in the GeV-regime, wakefield accelerator stages with lengths on the order of hundreds of millimeters are required (eg. Leemans et al., 2006). Propagating a high-intensity laser pulse over such distances in a plasma is difficult, since the pulse is attenuated rapidly due to diffraction and refraction. To achieve long attenuation lengths, laser pulses must be guided in a waveguide, a structure with a radially decreasing refractive index that results in a focussing effect. To this end, capillary discharge waveguides (Spence and Hooker, 2000; Butler et al., 2002) have been instrumental in achieving record electron energies with laser wakefield accelerators (Leemans et al., 2006). However, in such waveguides the support structure of the capillary is susceptible to laser damage, especially in an accelerator operated at high repetition rate. To overcome this limitation of capillary waveguides, Shalloo et al. (2018) have proposed the use of low density plasma channels created by optical-field-ionisation of a neutral gas column. An experimental campaign at the **Astra** laser facility of the Rutherford Appleton Laboratory

investigated the guiding of high-intensity laser pulses over long distances in such plasma channels (Shalloo et al., 2019; Picksley et al., 2020). The author participated in the day-to-day operation of the experiment, developed automatic components for control of optical elements under vacuum and performed fluid-dynamic modelling of the gas flow in the laser-plasma interaction region to predict plasma density profiles. The experiments successfully demonstrated guiding of a high-intensity pulse ($I = 4 \times 10^{17} \text{ Wcm}^{-2}$) over more than 14 Rayleigh ranges at a 5 Hz repetition rate (Shalloo et al., 2019), and showed that the plasma waveguide attenuation length can be extended to the meter scale if a conditioning pulse is used to ionise the neutral gas collar that surrounds the plasma channel (Picksley et al., 2020).

3.1.2 ION MOTION IN LASER WAKEFIELDS

The Oxford laser-plasma accelerator group has performed experiments that demonstrated the resonant excitation of wakefields with trains of laser pulses (Cowley et al., 2017, no contribution by the author of this thesis), using the **Astra-Gemini** TA2 laser facility at the Rutherford Appleton Laboratory. Trains of up to seven successive pulses were used to resonantly excite an electron density perturbation with relative amplitude $\delta n_e/n_{e0}$ on the order of 1%. Wakefields were measured via Frequency Domain Holography (FDH, Matlis et al., 2006) and temporally encoded spectral shifting (TESS, Matlis et al., 2016; Arran et al., 2018), that employ a long diagnostic laser pulse that co-propagates with the wakefield and phase-encodes the density oscillation associated with the Langmuir wave. The phase information can be recovered by interference in an imaging spectrometer of the diagnostic pulse with a reference pulse that propagates ahead of the wakefield. By performing a targeted damping of the wakefield using a trailing laser pulse, off-resonant with the

plasma frequency, the experiments by Cowley et al. (2017) also demonstrated the fine control over wakefield parameters afforded by the multi-pulse scheme. In the experiments by Cowley et al. (2017) it was also observed that the wakefield generated by the train of laser pulses decayed on a timescale comparable to the ion plasma period, indicating that on this timescale, interactions between the electron plasma oscillation and the plasma ions take place. In long pulse trains, the total duration of the pulse train may exceed the ion plasma period. In an electron-proton plasma, the mass ratio $m_e/m_i \approx 1/1836$ implies that $\omega_{pe}^{-1}/\omega_{pi}^{-1} \approx 1/43$. For a pulse train of $N \gtrsim 43$ pulses that are resonant with the plasma frequency one therefore expects ion dynamics to affect the laser wakefield. Particle-in-cell simulations by Hooker et al. (2014) confirm this estimate. Experiments at the Rutherford Appleton's **Gemini** facility to which the author contributed were performed to further investigate the decay process of laser wakefields, at higher wakefield amplitudes. These experiments generated wakefields with an amplitude on the order of 5 – 10% and measured the decay rate of the wakefields in plasmas with different ion masses. The experiments are described in detail in Jonnerby et al. (2021) and are briefly outlined here. A schematic of the experimental design is shown in Figure 3.5. The **Gemini** facility consists of a two-beam Titanium-doped Sapphire chirped-pulse-amplification (CPA) laser system, with an energy of 15 J, minimum pulse duration of 30 fs and peak intensity of $2 \times 10^{21} \text{ Wcm}^{-2}$, depending on the focussing optic that is employed. The temporally synchronised beams from the **Gemini** facility were used to measure the evolution of laser wakefields, as follows: The first beam (Beam 1) was passed through a second-harmonic generating crystal to double the laser frequency (SHG, shown in blue in Figure 3.5), then split into a reference pulse and diagnostic pulse in a Michelson interferometer. The reference and diagnostic pulses were temporally stretched and frequency chirped by propagating through a borosilicate (BK7) glass block.

Both pulses were then passed through a holed mirror (labelled M3 in Fig. 3.5) towards the interaction region. The second beam (Beam 2, shown in red) was compressed and inserted into the beamline via the mirror M3, then focussed into a gas cell target to generate a laser wakefield. After propagating through the gas cell target, the wakefield driving pulse (Beam 2) was then filtered out using a dichroic mirror (M4). The diagnostic pulse co-propagated with the wakefield to record the plasma density structure in the optical phase of the diagnostic pulse. The diagnostic and reference pulses continued downstream towards forward diagnostics, where the two pulses were interfered in an imaging spectrometer. To measure the temporal evolution of the wakefield amplitude, a delay stage was used to scan over the timing of the diagnostic pulse, relative to the driving pulse.

The amplitude of the plasma density variation associated with the wakefield was determined from the spectral interferogram using the TESS method (Matlis et al., 2016; Arran et al., 2018). Wakefield e-folding decay times of $(87 \pm 34)\tau_{pe}$ [$2.0 \pm 0.8\tau_{pi}$] and $(171 \pm 66)\tau_{pe}$ [$2.8 \pm 1.1\tau_{pi}$] were determined for hydrogen and deuterium plasmas, respectively, where τ_{pe} and τ_{pi} denote the electron and ion plasma periods. The measurements confirm that the wakefield decay time is on the order of the ion plasma period and indicate that the decay time depends on the mass of the plasma ions, suggesting that ion dynamics play an important role in the decay mechanism. Particle-in-cell (PIC) simulations performed by the author confirmed that if ion motion is artificially suppressed in the PIC simulations, corresponding to infinitely heavy ions, no decay of the laser wakefield occurs on the timescale of the ion plasma period. The dynamics of plasma ions in laser wakefields will be investigated in detail in Chapters 4 and 5.

3.2 TARGET DESIGN

In preparation for the experiments to measure the decay rate of laser wake-fields (Jonnerby et al., 2021) and for future experiments in the group, the author led the design of the gas cell target that provided the laser-plasma interaction region. This design is described in this section. Computer-aided designs (CAD) of the gas cell target developed by the author are shown in Figures 3.1 and 3.2. A pressurised gas flow through the cell is established to create an interaction region for laser-plasma experiments. Manufacture of the cell design and testing was performed in collaboration with the Clarendon Laboratory instrumentation workshop. Key design requirements of the target cell were flexible adjustment of the length of the laser-plasma interaction region, good optical access to the interaction region, a long operating lifetime, and easy maintenance of parts that are irradiated by high-intensity laser light. The exterior dimensions of the cell measure $30 \text{ mm} \times 15 \text{ mm} \times 15 \text{ mm}$. The cell interior can be pressurised to a specified pressure, to control the plasma density after ionisation. The gas feed begins at the back surface (right side in Figure 3.2) of the cell base, and is connected to the interaction region from below, centered between the two nozzles. Ultra-high vacuum stability of the cell was verified down to $1 \times 10^{-10} \text{ mbar}$ for closed nozzles using a helium probe to rule out leaks. Transverse windows enable on-shot imaging of the formed plasma, and can be used for transverse measurements in experiments that require these. The longitudinal scale length of the interaction region was set by the Rayleigh range of the laser beam, $z_R \sim 6.5 \text{ millimeters}$, for a $40 \mu\text{m}$ spot-size, 800 nm beam. To enable control over the length of the interaction region, three cell-length configurations were produced by varying the length of the rear cap that holds one of the nozzles: a sub- z_R , $L = 4 \text{ mm}$ configuration, a $L = 6 \text{ mm}$ configuration comparable to the Rayleigh range, and a long configuration, $L = 8 \text{ mm} > z_R$, where L denotes the distance between the nozzles.

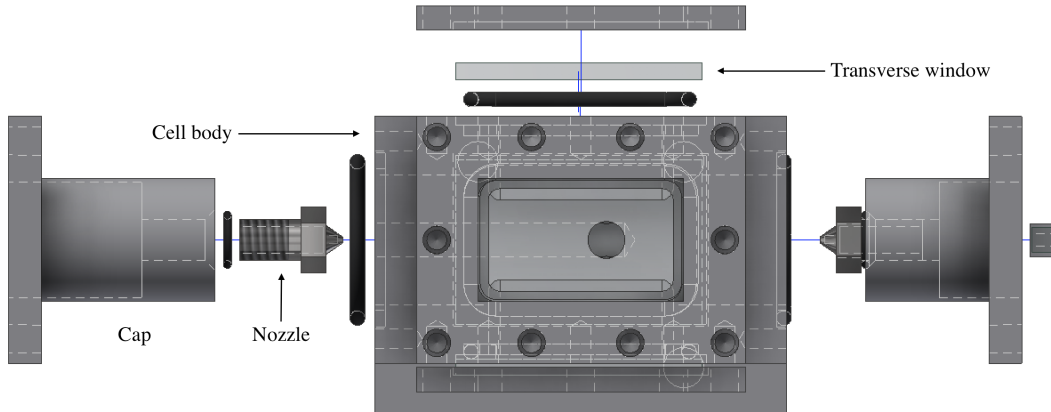


Figure 3.1: Partially exploded view of the gas-cell target. The cell is viewed from the top, and shows the nozzle mounting and a transverse window. Interior edges are indicated by dashed lines. The laser pulse is injected from the right and exits the cell on the left; the laser-plasma interaction takes place in the region between the two nozzles. The cell is pressurised via the gas-feed in the cell base.

In previous experiments in the group, including the guiding experiments described in Section 3.1.1, laser pulses were injected into the gas cell through stainless steel or Inconel pinholes, that were susceptible to laser damage and required frequent replacement. Compared to previous gas cells employed in the group, the cell design presented here makes use of off-the-shelf stainless steel extruder nozzles from high-temperature 3D printers. This design reduces the number of bespoke parts required for cell construction and maintenance and simplifies the assembly. The nozzles are bolted into the cell front and back caps, as shown in the magnification in Figure 3.2. The robustness of the nozzles to irradiation by high-intensity laser pulses was confirmed during the experiments at the Rutherford Appleton Laboratory described in Section 3.1.2.

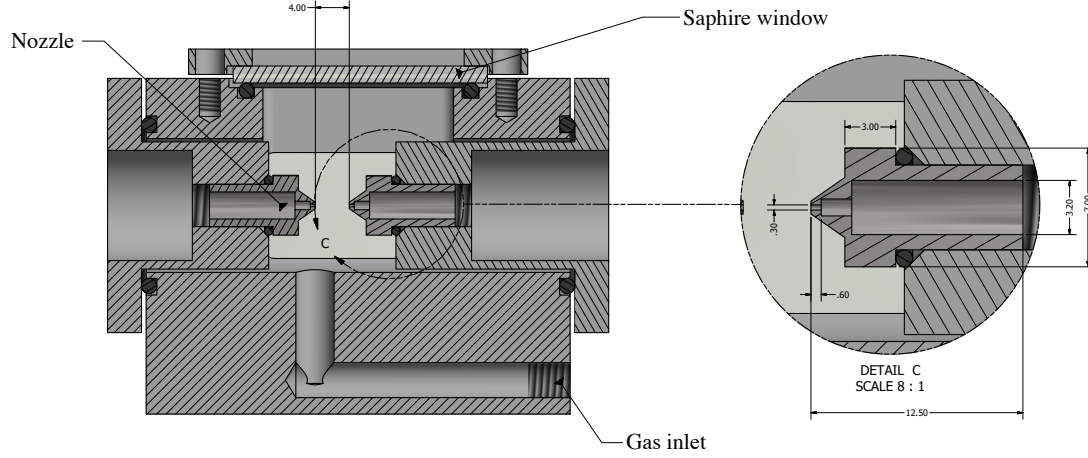


Figure 3.2: Cut view of the gas-cell target, viewed from the side. The laser pulse is injected from the right and exits the cell on the left; the laser-plasma interaction takes place in the region between the two nozzles. The cell is pressurised via the gas-feed in the cell base.

3.3 SIMULATION OF THE FLOW-PROFILE

The pressure profile of the gas-cell controls the plasma density profile after ionisation by the driving laser pulse. Knowledge of the pressure profile is therefore essential for the operation of a laser-wakefield accelerator, since the laser-plasma interaction itself, and the dynamics of the plasma electrons in the wakefield, are dependent on the plasma density, n_e , via the plasma frequency, $\omega_{pe} = (e^2 n_e / m_e \epsilon_0)^{1/2}$. For a multi-pulse laser wakefield accelerator in particular, the plasma period $\tau_{pe} = 2\pi / \omega_{pe}$, defines the pulse spacing required for the resonant excitation of a wakefield. The interaction between the laser beam and target plasma is also dependent on the density, since the refractive index, η , is dependent on the plasma density, $\eta = (1 - \omega_{pe}^2 / \omega^2)^{1/2} \sim 1 - \omega_{pe}^2 / 2\omega^2 = 1 - n_{e0} / 2n_c$, for $\omega_{pe} \ll \omega$, where ω denotes the angular frequency of the laser and $n_c = \epsilon_0 m_e \omega^2 / e^2$ denotes the critical plasma density. Variations in the plasma density thus affect the prop-

agation of the laser pulse, for instance via a focusing or defocusing effect. To prevent this, the gas density profile must be uniform. Knowledge of the density profile is also required for longitudinal measurements of the wakefield density structure using a co-propagating diagnostic pulse as described in Section 3.1.2, since the phase shift experienced by the diagnostic beam depends on the length of plasma traversed by the beam.

The gas cell was pressurised via a solenoid valve located in the target vacuum chamber and connected to the gas cell via a silicon feed. The valve was temporally synchronised to open immediately prior to an incident laser pulse. Sound speed estimates suggest that within milliseconds after valve opening a steady-state flow is established within the cell. The subsequent steady-state flow-profile in the gas-cell was characterised using the **OpenFOAM** computational fluid dynamics toolbox (Open Source Field Operation and Manipulation, Weller et al., 1998, <https://openfoam.org>). The **OpenFOAM** mesh-generator **BlockMesh** was used to create a 2D mesh of the gas cell cross-sectional geometry. To enable convenient variation of the mesh geometry, a **python** program was written by the author that automatically parses cell specifications into an input file for the **BlockMesh** mesh-generator.

During experimental operation, the pressurised gas cell is located in a vacuum chamber; as a result, a large pressure gradient between the cell interior and exterior drives a high-speed outflow. The **SonicFoam** solver was used to solve the compressible Navier-Stokes equations for high flow-speeds on the order of the sound-speed. The geometry of the simulation approximately reproduced the cross-sectional geometry of the cell interior and the inflow and outflow regions, with dead-spaces near the transverse and top windows, and in the clearances between the cell body and front and rear caps neglected to reduce the mesh complexity. These simplifications are far from the areas of high-speed flow and are therefore expected to have no significant effect on the steady-state

flow profile. The simulation geometry for a 4 mm cell is shown in Figure 3.3. Boundary conditions were set to establish the cell pressure at the gas inlet to the interior volume of the cell, P_i , and a vacuum pressure, P_v , at both outlets of the cell. The outlet pressure boundaries implement an anechoic boundary type that specifies a far-field pressure beyond the boundary and adapts the boundary pressure to prevent the reflection of pressure waves at a nonphysical "hard" pressure boundary. Boundary conditions for the flow velocity, u , were set such that $u = 0$ on all surfaces; this *no-slip condition* is justified by the formation of a boundary sheath on surfaces that is typical for viscous flow (Anderson, 2003). Boundary conditions for the derivative of the pressure field specify $\nabla P = 0$ on every surface. For the flow velocity, $\nabla u = 0$ was specified at the outlets. The gas temperature was set to 300 K on all surfaces, at the inlet and on the outlets. Initial conditions for the mesh interior were set to $u_0 = 0$, $P_0 = P_i$ and $T_0 = 300$ K. The complete domain was initialised at the inlet pressure P_i to avoid the numerically difficult simulation of the extremely fast filling process. An estimate of the significance of turbulence in the flow regime encountered here can be made from the ratio of the inertial to viscous forces, given by the Reynolds number, $Re = \rho u L / \mu \sim 1200$, where μ denotes the dynamic viscosity. Assuming a sonic flow of hydrogen at 100 mbar, a temperature of 300 K, and a characteristic length scale $L \sim 1$ mm associated with the cell geometry, then $Re \sim 1200$. At such high Reynolds numbers turbulence is significant, however, resolving the turbulence is numerically expensive. **OpenFOAM** permits a modeling of the effect of turbulence using the $k - \omega$ shear-stress transport (SST) model (Menter, 1994) to account for turbulent kinetic energy and its dissipation into heat. During a simulation, the Courant number, $c = u \Delta t / \Delta x$, was monitored, where Δt and Δx denote the timestep of the solver, and the size of the smallest cell in the mesh, respectively. For numerical stability, the Courant-Friedrichs-Lewy (CFL) condition

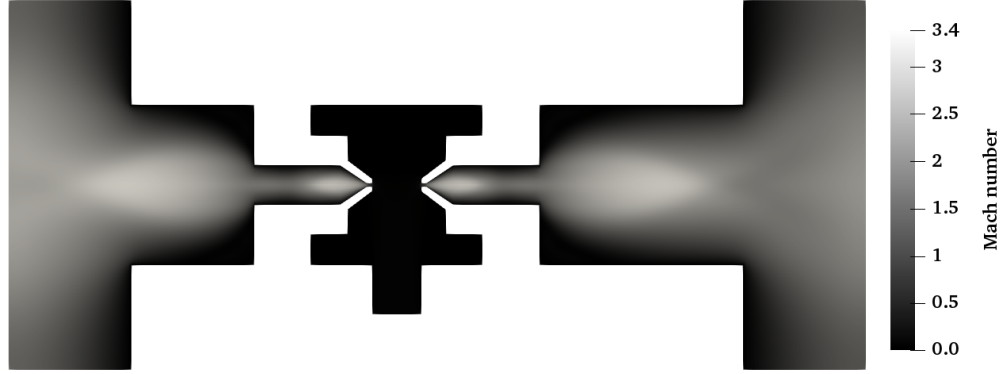


Figure 3.3: Simulation geometry and Mach number field for steady-state flow through the gas-cell target for a nozzle diameter $d = 0.25$ mm. A backing pressure $P_i = 1 \times 10^4$ Pa is applied at the central, lower cell inlet. A vacuum pressure far-field $P_v = 1 \times 10^{-6}$ Pa was specified on the left and right outflow boundaries.

requires that $c < 1$, such that the time discretization is small enough to temporally resolve the crossing of a cell in the mesh by a fluid element travelling with velocity u . The steady-state was identified by examining the profiles of the flow parameters at successive outputs of the simulation, and by monitoring the solver residuals as a function of the timestep. Figure 3.3 shows the steady-state flow profile via the Mach number field, Ma , the ratio of the flow-speed, u , to the local speed of sound, $c_s = (\gamma k_B T / m)^{1/2}$, with $\gamma = 1.4$ for diatomic hydrogen. Figure 3.3 indicates that at the outlets of the cell the flow is supersonic. The Mach number profile can be understood from a one-dimensional flow approximation: if the flow velocity is assumed to be independent of the radial coordinate, the fluid equations simplify and an area-velocity relation can be derived (Anderson, 2003). For a particle in a section of the flow that has a cross-sectional area A , one obtains

$$\frac{dA}{du} = [(Ma)^2 - 1] \frac{A}{u}, \quad (3.1)$$

where $Ma = u/c_s$ denotes the Mach number and u denotes the flow speed. For subsonic velocities, $Ma < 1$, the area velocity relation implies that a decrease

in the cross-sectional area of the flow causes an increase in the flow-speed. In the supersonic regime, $Ma > 1$, an increase in the area causes an increase in the flow-speed. This behavior is observed in the simulations: the constriction of the gas-flow in the nozzle entrance, and subsequent expansion in the nozzle neck and the capillaries accelerates the flow to supersonic velocities. The phenomenon is analogous to the acceleration of gases in converging-diverging de Laval geometries of rocket engines or supersonic wind tunnels. Weak oblique shocks are observed to form in the exhaust plume before the cap exit. The X-shape of these shocks, discernible in the right-hand cap, and absence of a normal shock front (Mach disk) are characteristic of moderately underexpanded supersonic jets propagating into a reservoir of lower ambient pressure (Norman et al., 1982; Ladenburg et al., 1949; Hartmann and Lazarus, 1941).

The gas density is proportional to the electron density after ionisation of the neutral gas by the laser pulse. Axial line-outs of the electron density, calculated from the flow pressure and temperature profile assuming complete ionisation of molecular hydrogen, are shown in Figure 3.4 for nozzle diameters of $d = 0.25$ mm, $d = 0.40$ mm and $d = 0.55$ mm. The cell is $l = 4$ mm long, and pressurized to $P_i = 1 \times 10^4$ Pa (100 mbar) at the inlet. For the 0.25 mm nozzles, the line-out indicates that for the central 3 mm of the cell, the density deviates from the set density by no more than 0.4%. Within this central region, the longitudinal uniformity of the electron density is excellent. In the vicinity of the nozzle openings, the density drops by 9% with respect to the set density. The electron density halves with respect to the set density after a distance of 0.35 mm from the nozzle front surfaces. For the 0.55 mm nozzle, the density halves after a distance of 0.40 mm after the front surface of the nozzle. Transverse line-outs of the density through the cell centre showed a negligible density variation on spatial scales on the order of the laser beam-width $w_0 \approx 40$ μ m. The gas cell target described here was used successfully

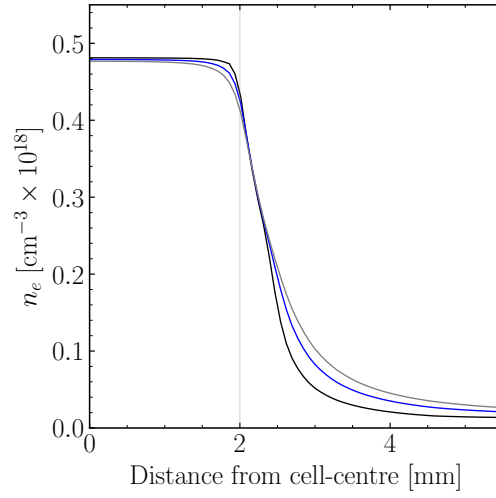


Figure 3.4: Axial density profile during steady-state gas flow for a 4 mm cell calculated from **OpenFOAM** simulations. The density profiles correspond to nozzle diameters of $d = 0.25$ mm (black), $d = 0.40$ mm (blue) and $d = 0.55$ mm (grey).

in experiments at the Rutherford Appleton Laboratory to measure the decay rate of laser wakefields, described in detail in Jonnerby et al. (2021).

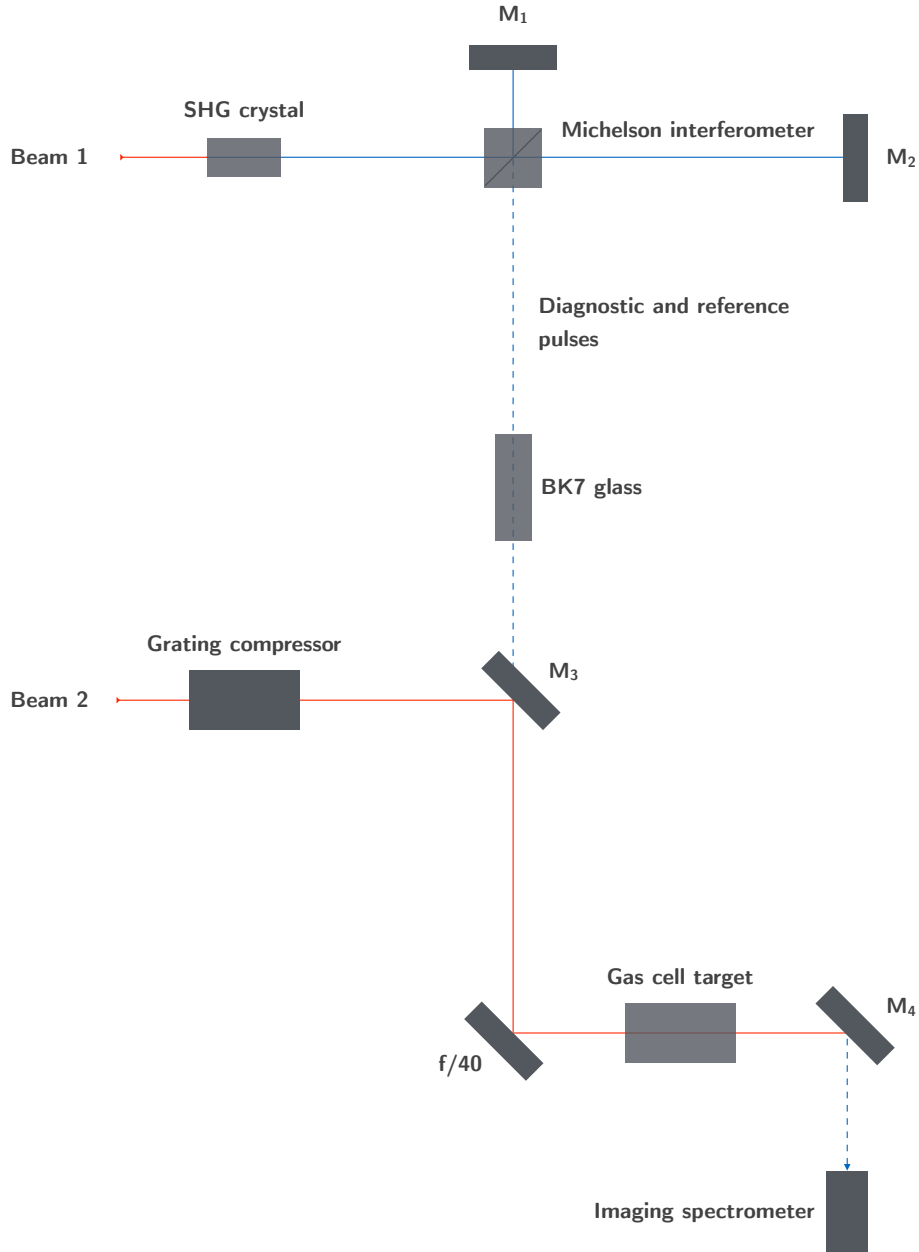


Figure 3.5: Schematic layout (not to scale) of an experiment to measure the temporal evolution of laser wakefields: Beam 1 is frequency-doubled and split into diagnostic and reference pulses that are co-axially injected with Beam 2. Beam 2 is used to drive a laser wakefield in a gas cell target. The reference and diagnostic pulses are interfered in an imaging spectrometer to measure the wakefield amplitude.

CHAPTER 4

STRONG-FIELD MODULATIONAL INSTABILITY

In this chapter, we review the theory of the modulational instability for electrostatic plasma oscillations, beginning with the weak-field regime (Zakharov, 1972) and then covering the strong-field regime (Silin, 1967; Sanmartin, 1970). The obtained dispersion relation will be used in the subsequent chapter for an interpretation of particle-in-cell simulations. Gaussian units are used in this chapter unless specified otherwise.

4.1 INTRODUCTION

Modulational instabilities are a ubiquitous phenomenon in nature and in laboratory physics, occurring, for instance, in surface water waves (Benjamin and Feir, 1967), in optical fibers (Tai et al., 1986), magnetised fusion plasmas (cf. Diamond et al., 2005) and plasma-based accelerators (Moulin et al., 1994). Fundamentally, the modulational instability is a four-wave interaction that can be understood in the spectral domain as follows: the interaction of a high-frequency carrier wave, (ω_0, k_0) , with a low-frequency wave, (Ω_s, k_s) , results in the formation of two sideband waves, $(\omega_{12} = \omega_0 \pm \Omega_s, k_{12} = k_0 \pm k_s)$, that have frequencies slightly shifted from the carrier wave frequency. The interaction

of the sideband waves with the carrier constitutes an amplitude modulation of the carrier wave that can couple to the low-frequency wave and lead to an unstable growth of the low-frequency and sideband wave amplitudes. In a plasma, a high-frequency Langmuir wave couples to slow perturbations of the ion density via the ponderomotive force: in regions of decreased ion density, the refractive index of the plasma is increased, leading to a focussing of Langmuir oscillations in such density depressions. The associated non-uniformity of the Langmuir wave envelope results in a ponderomotive force that acts to further enhance the ion density perturbation, leading to an instability. This phenomenon is considered in detail in the context of laser wakefields in the following sections. The development of the modulation instability in laser wakefields has been inferred in experiments (Moulin et al., 1994; Blanc et al., 1996; Ting et al., 1996; Marques et al., 1996; Kotaki et al., 2002), but few direct investigations of the instability or its effect in a wakefield exist that combine numerical studies and theory (Mora et al., 1988; Héron and Adam, 1993). We begin by reviewing the theory of the modulational instability in a plasma in regimes applicable to laser wakefield accelerators.

The interaction of Langmuir waves with the ion species of a plasma was first investigated in the context of weak plasma turbulence, leading to the discovery of a modulational ion instability that acts as a dissipation mechanism for Langmuir waves (Vedenov and Rudakov, 1964). In the limit of small Langmuir wave energy relative to the plasma thermal energy, the modulational instability is described by the Zakharov equations (Zakharov, 1972), that model the nonlinear interaction of a fast electrostatic oscillation and slow ion acoustic waves via the ponderomotive force. We sketch the derivation here following Zakharov (1972) and Thornhill and ter Haar (1978), because it is physically instructive, if only applicable for weak Langmuir waves. The derivation relies on a linearisation of the electron and ion fluid equations, by using the low

mass ratio of the plasma species ($\mu = m_e/m_i \approx 1/1836 \ll 1$ for a hydrogen plasma) to separate the plasma motion according to a short electron timescale, $\tau_e \sim \omega_{pe}^{-1}$, and a long ion timescale, $\tau_i \sim \omega_{pi}^{-1} \sim \tau_e(m_i/m_e)^{1/2} \gg \tau_e$. One may then decompose fluid quantities into components varying on the fast and slow timescales, respectively. We assume the presence of a high-frequency electrostatic plasma oscillation, with wave number k_0 and frequency ω_0 and a small perturbation of the ion density with wave number k , in an initially uniform plasma. Neglecting the ion response to the fast electron oscillations, the ion density evolves on the slow timescale $n_i = n_0 + \delta n_i$, where n_0 denotes the equilibrium plasma density and δn_i denotes a slowly varying ion density perturbation. The electron density has a slow component that matches the ion density to maintain quasineutrality of the plasma on the slow timescale, and a fast varying component δn_f , such that $n_e = n_0 + \delta n_s + \delta n_f$. The electron and ion fluid velocities and quantities occurring in Maxwell's equations are decomposed analogously. The timescale separation then motivates an averaging over the fast timescale $\langle x \rangle = 1/\tau \int_0^\tau x(t') dt'$, so that the average of quantities that vary on the fast time scale vanishes on the slow timescale. Subtracting the averaged electron fluid equation from the electron fluid equation, one obtains the fast component of the electron fluid equation (Thornhill and ter Haar, 1978)

$$\begin{aligned} \frac{\partial \mathbf{v}_f}{\partial t} + (\mathbf{v}_s \cdot \nabla) \mathbf{v}_f + (\mathbf{v}_f \cdot \nabla) \mathbf{v}_s + [(\mathbf{v}_f \cdot \nabla) \mathbf{v}_f - \langle (\mathbf{v}_f \cdot \nabla) \mathbf{v}_f \rangle] \\ + \frac{e \mathbf{E}_f}{m_e} - \frac{\gamma_e k_B T_e}{n_e m_e} \nabla \delta n_f = 0, \end{aligned} \quad (4.1)$$

where one may use Gauss' law $q_e \delta n_f = -\nabla \cdot \mathbf{E}_f / 4\pi$ to introduce the electric field in the pressure term, and it was assumed that the electrons are non-relativistic to neglect the magnetic component of the Lorentz force.

We now consider the relative magnitude of the different terms in equation (4.1). The magnitude of the fast component of the electron fluid velocity can

be estimated using the acceleration of an electron in the fast-varying electric field, over the timescale $\tau_f \sim \omega_{pe}^{-1}$:

$$v_f \sim \frac{eE_f}{m_e} \omega_{pe}^{-1} \sim W^{1/2} v_{th,e}, \quad (4.2)$$

where $v_{th,e} \sim (\gamma_e k_B T_e / m_e)^{1/2}$ denotes the electron thermal velocity and we have introduced the important parameter

$$W = \frac{1}{2} \frac{E_f^2}{4\pi n_e k_B T_e}. \quad (4.3)$$

The parameter W measures the ratio of the electrostatic energy of plasma oscillations to the thermal energy of the plasma, assuming that the ion temperature is negligible compared to the electron temperature. For a typical laser-ionised hydrogen plasma used in wakefield accelerators, the ion temperature is on the order of the gas temperature, $T_i \sim 300 \text{ K} \sim 0.03 \text{ eV} k_B^{-1}$; this is much lower than the electron temperature that is on the order of the ionization energy of hydrogen, $T_e \sim 10 \text{ eV} k_B^{-1}$, thus indeed $T_i \ll T_e$.

The slow motion of electrons and ions is on the order of the ion acoustic speed

$$v_s \sim c_s \sim v_{th,e} \mu^{1/2} \ll v_{th,e}, \quad (4.4)$$

where $c_s = (k_B T_e / m_i)^{1/2}$ denotes the ion sound speed and $\mu = (m_e / m_i) \ll 1$ is the electron-ion mass ratio. We can estimate the spatial derivatives of v_s and v_f using the wave numbers of the slow and fast oscillations $\nabla v_f \sim k_0 v_f$ and $\nabla v_s \sim k v_s$, respectively. The following ordering is then established in the fast timescale electron fluid equation

$$\begin{aligned} & \underbrace{\frac{\partial \mathbf{v}_f}{\partial t}}_{\sim W^{1/2} v_{th,e} \omega_{pe}} + \underbrace{(\mathbf{v}_s \cdot \nabla) \mathbf{v}_f}_{\sim \mu^{1/2} W^{1/2} (k_0 \lambda_D) v_{th,e} \omega_{pe}} + \underbrace{(\mathbf{v}_f \cdot \nabla) \mathbf{v}_s}_{\sim \mu^{1/2} W^{1/2} (k \lambda_D) v_{th,e} \omega_{pe}} \\ & + \underbrace{[(\mathbf{v}_f \cdot \nabla) \mathbf{v}_f - \langle (\mathbf{v}_f \cdot \nabla) \mathbf{v}_f \rangle]}_{\sim W (k_0 \lambda_D) v_{th,e} \omega_{pe}} + \underbrace{\frac{e \mathbf{E}_f}{m_e}}_{\sim W^{1/2} v_{th,e} \omega_{pe}} - \underbrace{\frac{e \gamma_e \lambda_D^2}{m_e} \nabla (\nabla \cdot \mathbf{E}_f)}_{\sim W^{1/2} (k_0 \lambda_D)^2 v_{th,e} \omega_{pe}} = 0. \end{aligned}$$

We have introduced the Debye length via $\omega_{pe}^2 \lambda_D^2 = k_B T_e / m_e \sim v_{th,e}^2$. If $W \ll 1$ we may retain only terms of order $W^{1/2}$ and drop the convective term nonlinear in $\mathbf{v}_f$. Given the small electron-ion mass ratio, the remaining convective terms may also be discarded since these are subdominant by a factor $\mu^{1/2}$.

Applying the same ordering in Maxwell's equations and combining these with the electron fluid equation, one obtains an equation for the fast varying component of the electric field:

$$\frac{\partial^2 \mathbf{E}_f}{\partial t^2} + c^2 \nabla \times (\nabla \times \mathbf{E}_f) - \gamma_e v_{th,e}^2 \nabla (\nabla \cdot \mathbf{E}_f) = - \left(1 + \frac{\delta n_s}{n_0} \right) \omega_{pe}^2 \mathbf{E}_f. \quad (4.5)$$

Equation (4.5) describes the evolution of the fast varying component of the electric field under the influence of slow density variations δn_s . To close this equation and obtain a system that describes the evolution of $\mathbf{E}_f$, we require an equation for δn_s ; this can be obtained by considering the component of the electron and ion fluid equations that varies on the slow timescale. Performing the time average of the electron fluid equation to eliminate the fast component one finds for the slow motion

$$\frac{\partial \mathbf{v}_s}{\partial t} + (\mathbf{v}_s \cdot \nabla) \mathbf{v}_s + \langle (\mathbf{v}_f \cdot \nabla) \mathbf{v}_f \rangle + \frac{e}{m_e} \mathbf{E}_s + \frac{e}{m_e c} \langle \mathbf{v}_f \times \mathbf{B} \rangle = - \frac{\gamma_e T_e}{n_0 m_e} \nabla \delta n_s, \quad (4.6)$$

where the magnetic field component of the Lorentz force has been retained since $\langle \mathbf{v}_f \times \mathbf{B} \rangle$ may be comparable to the small $\mathbf{E}_s$. From Maxwell-Faraday's equation $-\frac{\partial \mathbf{B}}{\partial t} = \nabla \times \mathbf{E}$ and the lowest-order approximation of equation (??), $\frac{\partial \mathbf{v}_f}{\partial t} = -\frac{e}{m_e} \mathbf{E}_f$ one obtains $\mathbf{B} = \frac{m_e}{e} \nabla \times \mathbf{v}_f$. The lowest order approximation for $\mathbf{v}_f$ is valid for wavelengths that are long compared to the Debye length, $k_0 \lambda_D \ll 1$. With $\mathbf{v}_f \times (\nabla \times \mathbf{v}_f) = \frac{1}{2} [\nabla (\mathbf{v}_f \cdot \mathbf{v}_f) - (\mathbf{v}_f \cdot \nabla) \mathbf{v}_f]$ it then follows that

$$\langle (\mathbf{v}_f \cdot \nabla) \mathbf{v}_f \rangle + \frac{e}{m_e c} \langle \mathbf{v}_f \times \mathbf{B} \rangle = \frac{1}{2} \langle \nabla (\mathbf{v}_f \cdot \mathbf{v}_f) \rangle \approx \frac{e^2}{2 m_e^2 \omega_{pe}^2} \nabla \langle \mathbf{E}_f^2 \rangle, \quad (4.7)$$

where we used $\mathbf{v}_f \approx e \mathbf{E}_f / m_e \omega_{pe}$. In equation (4.7) we recognise the ponderomotive force $\mathbf{F}_{\text{pond}} = -e^2 \nabla \langle E_f^2 \rangle / (4 m_e \omega_{pe}^2)$ from the introduction to particle

dynamics in a non-uniform, high-frequency laser field in Section 2.2. However, here the ponderomotive force is associated with the non-uniformity of the time-averaged Langmuir oscillation at the plasma frequency ω_{pe} . Combining these results, the slow component of the electron fluid equation is given by (Thornhill and ter Haar, 1978)

$$\frac{\partial \mathbf{v}_s}{\partial t} + (\mathbf{v}_s \cdot \nabla) \mathbf{v}_s + \frac{e}{m_e} \mathbf{E}_s + \frac{\gamma_e T_e}{n_0 m_e} \nabla \delta n_s = -\frac{e^2}{2m_e^2 \omega_{pe}^2} \nabla \langle \mathbf{E}_f^2 \rangle \quad (4.8)$$

Analogously, the slow component of the ion fluid equation is given by

$$\frac{\partial \mathbf{v}_i}{\partial t} + (\mathbf{v}_i \cdot \nabla) \mathbf{v}_i - \frac{e}{m_i} \mathbf{E}_s + \frac{\gamma_i T_i}{n_0 m_i} \nabla \delta n_i = -\frac{m_e^2}{m_i^2} \frac{e^2}{2m_e^2 \omega_{pe}^2} \nabla \langle \mathbf{E}_f^2 \rangle. \quad (4.9)$$

Note that the acceleration of the ions due to the ponderomotive force is small by a factor m_e^2/m_i^2 compared to the acceleration of the electrons. With $v_s \approx v_i$ and $\delta n_s \approx \delta n_i$ and combining Eqs. (4.8) and (4.9) to eliminate the slow component of the electric field, one obtains (Thornhill and ter Haar, 1978)

$$\frac{\partial \mathbf{v}_s}{\partial t} + (\mathbf{v}_s \cdot \nabla) \mathbf{v}_s + c_s^2 \nabla \frac{\delta n_s}{n_0} = -\frac{1}{m_i} \frac{e^2}{2m_e^2 \omega_{pe}^2} \nabla \langle \mathbf{E}_f^2 \rangle \quad (4.10)$$

where we have used $T_i \ll T_e$ and $m_e \ll m_i$ to approximate the ion acoustic speed $c_s^2 = (\gamma_e T_e + \gamma_i T_i)/(m_e + m_i) \approx \gamma_e T_e/m_i$. Combining equation (4.10) with the ion continuity equation

$$\frac{\partial \delta n_s}{\partial t} + \nabla \cdot [(n_0 + \delta n_s) \mathbf{v}_s] = 0, \quad (4.11)$$

one obtains, linearly in δn_s and v_s

$$\left[\frac{\partial^2}{\partial t^2} - c_s^2 \Delta \right] \frac{\delta n_s}{n_0} = \frac{1}{8\pi n_0 m_i} \Delta \langle \mathbf{E}_f^2 \rangle, \quad (4.12)$$

where $\Delta := \nabla^2$ and we have used $n_0 = m_e \omega_{pe}^2/(4\pi e^2)$. Equation (4.12) completes equation (4.5) by describing the slow evolution of the plasma density, δn_s , through ion acoustic waves that are driven by the slowly varying electric field set up due to the ponderomotive force acting on electrons. Equations (4.5) and (4.12) can be simplified by introducing a complex envelope of the

fast electric field component via $\mathbf{E}_f = [\tilde{\mathbf{E}} \exp(-i\omega_{pe}t) + \tilde{\mathbf{E}}^* \exp(i\omega_{pe}t)]/2$ (Zakharov, 1972; Thornhill and ter Haar, 1978), where $\tilde{\mathbf{E}}$ describes the field envelope varying slowly in time and the exponential factors account for the fast temporal oscillations of the field at the electron plasma frequency. One then obtains the Zakharov equations for the evolution of the electric field envelope $\tilde{\mathbf{E}}$ due to slow plasma density variations δn_s

$$-2i\omega_{pe} \frac{\partial \tilde{\mathbf{E}}}{\partial t} + c^2 \nabla \times (\nabla \times \tilde{\mathbf{E}}) - \gamma v_{th,e}^2 \Delta \tilde{\mathbf{E}} = -\frac{\delta n_s}{n_0} \omega_{pe}^2 \tilde{\mathbf{E}}, \quad (4.13)$$

and the self-consistent evolution of the slow density variation due to the ponderomotive force associated with perturbations of the electric field envelope

$$\left[\frac{\partial^2}{\partial t^2} - c_s^2 \Delta \right] \frac{\delta n_s}{n_0} = \frac{1}{16\pi n_0 m_i} \Delta |\tilde{\mathbf{E}}|^2. \quad (4.14)$$

For a Langmuir wave, that is purely longitudinal, the second term in Eq. (4.13) vanishes, yielding the electrostatic Zakharov system. The Zakharov equations (4.13–4.14) can be used to analyse the stability of the plasma by considering a perturbation of the electric field and linearising the equations. Zakharov (1972) showed that for a monochromatic Langmuir wave the plasma density and Langmuir wave envelope are subject to an instability that has a maximum growth rate for wave numbers comparable to, or larger than the wave number of the Langmuir wave. As a result, the initially uniform Langmuir wave envelope is modulated. Crucially, the derivation of the Zakharov equations relied on the assumption $W \ll 1$ to neglect the non-linear terms in the electron fluid equation (4.1). The Langmuir waves of laser wakefield accelerators typically have wave energies far in excess of the plasma thermal energy, so that $W \gg 1$, precluding the applicability of the Zakharov model. Analytical investigations of this strong-field regime using small mass-ratio approximations were performed by Silin (1965, 1967) and Sanmartin (1970). These showed that the modulational instability persists, with a modified growth rate, for large-amplitude Langmuir waves. We review the investigation by Silin (1967) and Sanmartin (1970) in the following section.

4.2 THE SILIN-SANMARTIN DISPERSION RELATION

The stability of large-amplitude ($W \gg 1$) high-frequency electrostatic plasma waves was investigated by Silin (1965, 1967) and Sanmartin (1970). Both rely on expansions in the small electron-to-ion mass ratio. Silin's derivation of the dispersion relation of the strong-field modulational instability (SFMI) from the fluid equations is followed here. A cold, non-relativistic electron-ion plasma is assumed. The fluid equations for the electron and ion species are then

$$\frac{\delta n_\alpha}{\delta t} + \nabla(n_\alpha \mathbf{v}_\alpha) = 0 \quad (4.15)$$

$$\frac{\partial \mathbf{v}_\alpha}{\partial t} + \mathbf{v}_\alpha \cdot \nabla \mathbf{v}_\alpha = \frac{q_\alpha}{m_\alpha} \mathbf{E}, \quad (4.16)$$

where the species index α denotes electrons or ions. Given an electrostatic oscillation with spatially uniform field $\mathbf{E}_0$ and frequency ω_0 , the equilibrium velocity of the plasma species is

$$\mathbf{u}_\alpha = -\frac{q_\alpha}{m_\alpha \omega_0} \mathbf{E}_0 \cos \omega_0 t. \quad (4.17)$$

Linearising around the equilibrium oscillation velocity $\mathbf{u}_\alpha$, and species densities, $n_{0\alpha}$, and combining the fluid equations with Gauss' law, $\nabla \cdot \mathbf{E} = 4\pi \sum_\alpha q_\alpha n_\alpha$, one obtains (Silin, 1965)

$$\left[\frac{\partial}{\partial t} + \mathbf{u}_\alpha \cdot \nabla \right]^2 \delta n_\alpha = -4\pi \frac{q_\alpha n_{0\alpha}}{m_\alpha} \sum_\beta q_\beta \delta n_\beta, \quad (4.18)$$

where the sum over β runs over all species. We assume small perturbations of the density from the equilibrium, δn_α , proportional to $e^{i\mathbf{k} \cdot \mathbf{r}}$ to make the replacement $\mathbf{u}_\alpha \cdot \nabla \rightarrow i\mathbf{k} \cdot \mathbf{u}_\alpha$ above. The form of equation (4.18) suggests the ansatz (Silin, 1965)

$$\delta n_\alpha = \nu_\alpha(t) \exp \left(i \frac{q_\alpha}{m_\alpha \omega_0^2} \mathbf{k} \cdot \mathbf{E}_0 \sin \omega_0 t + i\mathbf{k} \cdot \mathbf{r} \right). \quad (4.19)$$

Substituting this ansatz, the functions $\nu_{(e/i)}$ are determined by

$$\frac{\partial^2 \nu_e}{\partial t^2} + \omega_{pe}^2 [\nu_e + \nu_i \exp(-ia \sin \omega_0 t)] = 0 \quad (4.20)$$

$$\frac{\partial^2 \nu_i}{\partial t^2} + \omega_{pi}^2 [\nu_i + \nu_e \exp(+ia \sin \omega_0 t)] = 0, \quad (4.21)$$

where, $a = \frac{1}{\omega_0^2} \left(\frac{e}{m_e} - \frac{eZ_i}{m_i} \right) \mathbf{k} \cdot \mathbf{E}_0 \approx e\mathbf{k} \cdot \mathbf{E}_0 / (m_e \omega_0^2)$ if the electron to ion mass ratio is small and the ion charge is not large, which will be assumed henceforth. The quantity a is then approximately equal to the ratio of the electron excursion distance in the oscillating electric field $\mathbf{E}_0$, to the wavelength of the mode, $2\pi k^{-1}$. Using the Jacobi-Anger expansion, the exponential coefficients in the system of equations (4.20) and (4.21) can be written as

$$\exp(ia \sin \omega_0 t) = \sum_{n=-\infty}^{+\infty} J_n(a) \exp(in\omega_0 t), \quad (4.22)$$

where $J_n(a)$ is the Bessel function of the first kind of degree n . The system of equations (4.20) and (4.21) therefore contains every harmonic of the equilibrium oscillation frequency, motivating the ansatz

$$\nu_e = \exp(\gamma t) \sum_{l=-\infty}^{\infty} u_l \exp(-il\omega_0 t), \quad \nu_i = \exp(\gamma t) \sum_{l=-\infty}^{\infty} w_l \exp(il\omega_0 t), \quad (4.23)$$

where the factor $\exp(\gamma t)$ accounts for growth or decay of the perturbation. Substituting this ansatz in equations (4.20) and (4.21), and requiring that the equations are satisfied for each harmonic one obtains equations for the coefficients u_l and w_l :

$$u_m = -\omega_{pe}^2 [\omega_{pe}^2 + (\gamma - im\omega_0)^2]^{-1} \sum_{l=-\infty}^{\infty} w_l J_{m+l}(a) = 0 \quad (4.24)$$

$$w_m = -\omega_{pi}^2 [\omega_{pi}^2 + (\gamma + im\omega_0)^2]^{-1} \sum_{l=-\infty}^{\infty} u_l J_{m+l}(a) = 0 \quad (4.25)$$

We now specialise to an external frequency at resonance with the plasma frequency, $n\omega_0 = \omega_{pe}$, $n \in \mathbb{Z}$; in the context of laser wakefields we will be

interested in $n = 1$. For small damping or growth the near-resonant denominators imply that $u_{m=\pm n} \gg u_{m \neq n}$. Ion modes with $m \neq 0$ are small compared to the resonant electron modes, by a factor $\omega_{pi}^2/\omega_{pe}^2 = \mu \ll 1$. Retaining only the fundamental w_0 -ion mode, and the resonant $u_{m=\pm n}$ electron modes, one obtains (Silin, 1965)

$$w_{m \neq 0} = -\frac{\mu\omega_{pe}^2}{\omega_{pi}^2 + (\gamma + im\omega_0)^2} \left[u_n J_{m+n} + u_{-n} J_{-n+m} - w_0 \sum_{l \neq 0} \frac{\omega_{pe}^2}{\omega_{pe}^2 + (\gamma - il\omega_0)^2} J_l J_{l+m} \right] + O(\mu^2). \quad (4.26)$$

Using this in the expression for u_m one obtains

$$u_{m \neq n} = -\frac{\omega_{pe}^2}{\omega_{pe}^2 + (\gamma - im\omega_0)^2} \left[w_0 J_m - \sum_{l \neq 0} J_{l+m} \frac{\mu\omega_{pe}^2}{\omega_{pi}^2 + (\gamma + il\omega_0)^2} \times \left(u_n J_{l+n} + u_{-n} J_{-n+l} - w_0 \sum_{k \neq 0} \frac{\omega_{pe}^2}{\omega_{pe}^2 + (\gamma - ik\omega_0)^2} J_k J_{k+l} \right) \right] + O(\mu^2), \quad (4.27)$$

where we have dropped the argument of the Bessel functions for brevity. Retaining only first-order terms in the electron-ion mass ratio, and using these approximations in equations (4.24) and (4.25) for $u_{\pm n}$ and w_0 , one finds

$$u_n = -\frac{\omega_{pe}^2}{\omega_{pe}^2 + (\gamma - im\omega_0)^2} \left[w_0 J_n - \sum_{l \neq 0} J_{n+l} \frac{\mu\omega_{pe}^2}{\omega_{pi}^2 + (\gamma + im\omega_0)^2} \times \left(u_n J_{l+n} + u_{-n} J_{-n+l} - w_0 \sum_{k \neq 0} \frac{\omega_{pe}^2}{\omega_{pe}^2 + (\gamma - ik\omega_0)^2} J_k J_{k+l} \right) \right], \quad (4.28)$$

and

$$w_0 = -\frac{\omega_{pi}^2}{\omega_{pi}^2 + \gamma^2} \left[u_n J_n + u_{-n} J_{-n} - \sum_{l \neq \pm n} J_l \frac{\omega_{pe}^2}{\omega_{pe}^2 + (\gamma - il\omega_0)^2} \times \left\{ w_0 J_m - \sum_{l \neq 0} J_{l+m} \frac{\mu\omega_{pe}^2}{\omega_{pi}^2 + (\gamma + il\omega_0)^2} \times \left(u_n J_{l+n} + u_{-n} J_{-n+l} - w_0 \sum_{k \neq 0} \frac{\omega_{pe}^2}{\omega_{pe}^2 + (\gamma - ik\omega_0)^2} J_k J_{k+l} \right) \right\} \right]. \quad (4.29)$$

We have thus obtained a system of three equations for w_0 and $u_{\pm n}$ that we may rewrite as

$$u_{\pm n} \left[1 + \left(\frac{\gamma \mp in\omega_0}{\omega_{pe}} \right)^2 - \mu A_{\pm n} \right] - u_{\mp n} \mu B_{\pm n} + w_0 (J_{\pm n} + \mu C_{\pm n}) = 0, \quad (4.30)$$

and

$$w_0 \left[1 + \left(\frac{\gamma}{\omega_{pi}} \right)^2 - D_n + \mu E_n \right] + u_n (J_n + \mu C_n) + u_{-n} (J_{-n} + \mu C_{-n}) = 0, \quad (4.31)$$

where for compactness we have introduced the definitions (Silin, 1965)

$$A_n := \sum_{l \neq 0} J_{l+n}^2 \frac{\omega_{pe}^2}{\omega_{pi}^2 + (\gamma + il\omega_0)^2} \quad (4.32)$$

$$B_n := \sum_{l \neq 0} J_{l+n} J_{l-n} \frac{\omega_{pe}^2}{\omega_{pi}^2 + (\gamma + il\omega_0)^2} \quad (4.33)$$

$$C_n := \sum_{l \neq 0} \frac{\omega_{pe}^2}{\omega_{pi}^2 + (\gamma + il\omega_0)^2} \sum_{k \neq \pm n} \frac{\omega_{pe}^2}{\omega_{pe}^2 + (\gamma - ik\omega_0)^2} J_{n+l} J_k J_{k+l} \quad (4.34)$$

$$D_n := \sum_{l \neq \pm n} J_l^2 \frac{\omega_{pe}^2}{\omega_{pe}^2 + (\gamma + il\omega_0)^2} \quad (4.35)$$

$$E_n := \sum_{l \neq \pm n} \sum_{k \neq \pm n} \sum_{j \neq 0} \frac{-\omega_{pe}^6 J_l J_k J_{l+j} J_{k+j}}{[\omega_{pe}^2 + (\gamma + il\omega_0)^2][\omega_{pe}^2 + (\gamma + ik\omega_0)^2][\omega_{pi}^2 + (\gamma + ij\omega_0)^2]}. \quad (4.36)$$

Using the smallness of the electron-to-ion mass ratio, the infinite system of equations (4.24) and (4.25) is thus reduced to a closed system of three equations (4.30) and (4.31) for the three dominant perturbed modes in the plasma. The equations describe a four-wave interaction of three Langmuir modes (including the equilibrium oscillation) and one ion mode. To investigate the stability of the system, we set the determinant equal to zero and solve for the growth rates. The resulting expression is somewhat unwieldy (Silin, 1965) but can be simplified for certain special cases. For growth rates that are small compared to the electron plasma frequency $|\gamma| \ll \omega_0, \omega_{pe}$, and sharp resonance of

the equilibrium oscillation with the plasma frequency, $\lambda := |1 - n^2 \omega_0^2 / \omega_{pe}^2| \ll 1$, one obtains an equation for the normalised growth rate $\tilde{\gamma} := \gamma / \omega_{pe}$ (Silin, 1965)

$$\begin{aligned} \tilde{\gamma}^4 + \tilde{\gamma}^2 \left[\frac{1}{4} \lambda^2 + \mu \left(1 - D_n^0 - \frac{1}{2} J_n^2 - \frac{1}{2} \lambda A_n^0 \right) \right] + \frac{1}{4} \mu \left[\lambda^2 (1 - D_n^0) - 2 \lambda J_n^2 \right. \\ \left. + \mu \left\{ 2 J_n^2 [A_n^0 - (-1)^n B_n^0] + \lambda [-4 J_n C_n^0 + 2 A_n^0 (D_n^0 - 1)] \right\} \right] = 0. \end{aligned} \quad (4.37)$$

Here $A_n^0 = n^2 \sum_{l \neq 0} J_{l+n}^2 / l^2$ and the approximations B_n^0 , C_n^0 and D_n^0 are obtained analogously by using $\gamma \ll \omega_0$ to neglect γ and $\mu \ll 1$ (Silin, 1965). Equation (4.37) can be simplified further, depending on the size of the argument of the Bessel functions, a . For $a \sim 1$ one finds (Silin, 1965)

$$\tilde{\gamma}^2 = \frac{1}{2} \left[\beta \pm \left(\beta^2 + 2 \mu J_n^2 [\lambda - \mu (A_n^0 - (-1)^n B_n^0)] \right)^{\frac{1}{2}} \right] \quad (4.38)$$

where for compactness we have defined $\beta := \frac{1}{4} \lambda^2 + \mu (1 - D_n^0 - \frac{1}{2} J_n^2)$. In the special case $n = 1$, resembling an external field oscillating at the plasma frequency, the Bessel series in A_1^0 , B_1^0 and D_1^0 can be summed to obtain

$$A_1^0 - (-1)^1 B_1^0 = \sum_{l \neq 0} \frac{1}{l^2} [J_{l+1}^2 + J_{l+1} J_{l-1}] = \frac{2}{a^2} [1 - J_0^2], \quad (4.39)$$

$$1 - D_1^0 - \frac{1}{2} J_1^2 = 1 - \frac{2}{a} J_0 J_1, \quad (4.40)$$

where we have used standard identities for integer-order Bessel functions, and the identity given in the appendix to Sanmartin (1970). The dispersion relation is then

$$\begin{aligned} \tilde{\gamma}^2 = \frac{1}{2} \left[\frac{1}{4} \lambda^2 + \mu \left(1 - \frac{2}{a} J_0 J_1 \right) \pm \left\{ \left[\frac{1}{4} \lambda^2 + \mu \left(1 - \frac{2}{a} J_0 J_1 \right) \right]^2 \right. \right. \\ \left. \left. + 2 \mu J_1^2 \left[\lambda - \frac{2}{a^2} \mu (1 - J_0^2) \right] \right\}^{\frac{1}{2}} \right] \end{aligned} \quad (4.41)$$

The derivation of the dispersion relation (4.41) has assumed a cold plasma; as a result electrons and ions can oscillate at their respective plasma frequencies, ω_{pe} and ω_{pi} . Sanmartin (1970) performed a derivation of the dispersion relation for non-zero electron and ion temperatures. If the external frequency

is large compared to the ion plasma frequency, $\omega_0 \gg \omega_{pi}$, and wavelengths are long compared to the electron Debye length, $k\lambda_{D,e} = kv_{th,e}/\omega_{pe} \ll 1$ the complicated general dispersion relation obtained by Sanmartin (1970) can be simplified. For a laser wakefield, that oscillates at the plasma frequency, the resonance parameter $\tilde{\lambda} := (\omega_0^2 - \omega_{ke}^2)/\omega_{pe}^2 \ll 1$ is then small, where $\omega_{ke}^2 = \omega_{pe}^2 + 3k^2v_{th,e}^2$. With $\mu := m_e/m_i \ll 1$, the dispersion relation is then approximately given by (Sanmartin, 1970)

$$1 + \chi_i^0(\gamma/kv_{th,i}) \left[1 - 2 \frac{J_0(a)J_1(a)}{a} + k^2\lambda_D^2 - 2J_1(a)^2 \frac{\tilde{\lambda} - \frac{1}{4}\tilde{\nu}^2 + 2\mu[1 - J_0(a)^2]a^{-2}}{\tilde{\lambda}^2 + (2\tilde{\gamma} + \tilde{\nu})^2} \right] = 0, \quad (4.42)$$

where $\tilde{\gamma} = \gamma/\omega_{pe}$ denotes the normalised growth rate and

$$\tilde{\nu} = \nu/\omega_{pe} \approx (\pi/2)^{1/2}(k\lambda_D)^{-3} \exp\left(-\frac{1}{2k^2\lambda_D^2}\right) \quad (4.43)$$

is the normalised Landau damping rate. The ion susceptibility χ_i^0 can be related to the plasma dispersion function for a Maxwellian plasma. The assumption $k\lambda_D \ll 1$ implies for $T_i/T_e \ll 1$ that $kv_{th,i} = \omega_{pi}k/k_i \ll \omega_{pi}$. It follows that for instabilities with growth timescales $\gamma^{-1} \sim \omega_{pi}^{-1}$ – which we will encounter in the next chapter – the ion susceptibility can be approximated using the large argument asymptotic expansion of the plasma dispersion function (Fried and Conte, 1961), to first order $\chi_i(\gamma/kv_{th,i}) \approx \omega_{pi}^2/\gamma^2$, to obtain the quartic equation

$$\left[\tilde{\lambda}^2 + (2\tilde{\gamma} + \tilde{\nu})^2 \right] \left[\tilde{\gamma}^2 + \mu \left(1 - \frac{2}{a} J_0(a)J_1(a) \right) \right] - 2\mu J_1^2(a) \left[\tilde{\lambda} - \frac{1}{4}\tilde{\nu}^2 + 2\mu[1 - J_0(a)^2]a^{-2} \right] = 0. \quad (4.44)$$

where $\lambda(k) = (\omega_{ke}^2 - \omega_0^2)/\omega_{pe}^2 = 1 + 3k^2\lambda_D^2 - \omega_0^2/\omega_{pe}^2$, with $\omega_{ke}^2 = \omega_{pe}^2 + 3k^2v_{th,e}^2$. The finite electron temperature has modified the Silin dispersion relation to include the effect of Landau damping and modified the resonance parameter, λ , via the temperature dependence of the Bohm-Gross dispersion relation for

Langmuir waves. By setting $kv_{th,e} = 0$ in equation (4.44) one recovers the result of Silin for a cold plasma (4.41). The dispersion relation (4.44) is valid provided that the growth rate of any instability is small compared to the frequency of the driving wave $\gamma \ll \omega_0$, that the driving wave is in resonance with the plasma frequency, $\omega_0 \approx \omega_{pe}$, and that the wavelength of any mode is large compared to the Debye length $k\lambda_D \ll 1$, which implies $kv_{th,e} \ll \omega_0$. In the following chapter, we use the dispersion relation obtained here together with particle in cell simulations to investigate the dynamics of ions in laser wakefields.

CHAPTER 5

PARTICLE IN CELL SIMULATIONS

In this chapter, we use two-dimensional, Debye-scale resolution particle in cell simulations to investigate the ion dynamics in large-amplitude, linear laser wakefields. Comparisons of the simulation results with an analytic theory of the strong-field modulational instability reviewed in Chapter 4 are performed, and the implications of the findings for multi-pulse laser wakefield accelerators are discussed.

5.1 THE PARTICLE IN CELL METHOD

Particle in cell codes are an indispensable tool in the computational simulation of plasmas. Since a plasma consists of many individual particles, direct simulation of the particle dynamics in six-dimensional position-velocity $(\mathbf{x}, \mathbf{v})$ phase space is intractable. The equation of motion of the plasma particles is governed by the Lorentz force

$$\frac{d\mathbf{x}}{dt} = \mathbf{v} \tag{5.1}$$

$$\frac{d\mathbf{v}}{dt} = \frac{q}{\gamma m} [\mathbf{E} + \mathbf{v} \times \mathbf{B}], \tag{5.2}$$

where $\gamma = 1/\sqrt{1 - v^2/c^2}$ is the relativistic Lorentz factor and m denotes the rest mass. It follows from equation (5.2) that the acceleration of a particle

scales with q/m – as a result, a particle of charge Nq and mass Nm moves in the same way as a particle with charge q and mass m . This insight motivates the particle in cell (PIC) method: individual plasma particles are collected into macroparticles with total charge and mass equal to the sum of the contained particles' charges and masses. A PIC code reduces the computational complexity by simulating a plasma consisting of such macroparticles. The positions and velocities of each macroparticle are evolved in time by numerically integrating the equation of motion. At each time step, the electric and magnetic fields in the Lorentz force equation are determined by Maxwell's equations:

$$\nabla \cdot \mathbf{B} = 0 \quad (5.3)$$

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \quad (5.4)$$

$$\frac{1}{\mu_0} \nabla \times \mathbf{B} = \mathbf{j} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} \quad (5.5)$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}. \quad (5.6)$$

The electric and magnetic fields are calculated on a discrete spatial grid that gives rise to the eponymous spatial cell structure of particle in cell codes. The charge and current densities in the Maxwell equations, ρ and $\mathbf{j}$, respectively, are calculated at grid points by summing the charge and current contributions from particles in cells surrounding the grid points. The electromagnetic fields required at the macroparticle locations within cells to advance the particle position and velocity are obtained by interpolation between grid points. During the time advance of the PIC code, a single timestep thus consists of the following procedure: the fields are interpolated at the particle positions and are used to 'push' the particles to their new positions and velocities by integrating the equation of motion. The new charge and current densities are then calculated at the grid points, and Maxwell's equations are solved for the new electromagnetic fields. The code then proceeds iteratively.

Macroparticles have an associated *shape function*, to account for a finite spatial extent of the cloud of physical particles that is modelled collectively by a single macroparticle. The fidelity of a PIC simulation can be improved by increasing the number of macroparticles or by increasing the resolution of the time and space discretisations. Since the charge and current densities, and by extension the electromagnetic fields, rely on a summation of the contributions of macroparticles, a low number of macroparticles results in high noise levels. An important parameter for PIC simulations is the Debye length: if the Debye length is not resolved by the spatial discretisation in the simulation, spurious numerical heating of the plasma occurs, leading to an increase in the Debye length until this is resolved (cf. Cormier-Michel et al., 2008).

The simulations of laser wakefields discussed in this section were performed with the relativistic particle in cell codes **EPOCH** (cf. Arber et al., 2015) and **smilei** (Simulation of Matter Irradiated by Light at Extreme Intensities, Derouillat et al., 2018). Initial exploratory simulations were performed with **EPOCH**; the simulation results presented here relied exclusively on **smilei**, an open-source particle in cell code dedicated to the simulation of laboratory or astrophysical plasmas in general, with specific features optimised for the treatment of laser-plasma interactions, in particular. The code is also configured so as to perform well on massively parallel supercomputers. To parallelise a PIC simulation, the simulation domain is typically decomposed into computational regions that are aligned with the numerical grid and that are distributed across the nodes of the compute infrastructure. The code makes use of a variation of this method by splitting the domain into many small patches and distributing groups of patches between the nodes. Communication between nodes required for parallelisation is handled via the Message Passing Interface (MPI). The advantage of having a number of patches treated by each node lies in load balancing: patches can be moved between nodes to ensure

that the computational load of all nodes is approximately equal, thus avoiding situations in which nodes are idle, waiting for other nodes to complete computations. To minimise the overhead associated with communications between patches that are not part of the same node, `smilei` distributes patches along a Hilbert curve (Derouillat et al., 2018). Further parallelisation within a node is achieved by handling individual patches using OpenMP threads. The combination of these parallelisations and dynamic load balancing make `smilei` highly effective on massively parallel supercomputers. Usefully, the code provides a user-friendly diagnostic to verify that the computational load between patches is well balanced at all times in a simulation.

5.2 SIMULATION SETUP

The simulations presented here were performed on the ARCHER UK national supercomputing service and the Oxford Advanced Research Computing (ARC) cluster. Simulation parameters and code settings were optimized over a series of low-resolution, low particle-per-cell runs and then used for Debye-resolution, high-PPC simulations. Scans were used to determine that 64 PPC provide an acceptable noise level and numerical heating over the simulation timescale. The longitudinal resolution was set to the Debye length of the plasma so that Landau damping at small scales is accurately captured; the transverse resolution was limited to one-fifth of the longitudinal resolution by the available computational resources. A scan in the transverse resolution was performed, and the initial amplitude of the excited wakefield and evolution of the wakefield amplitude over several picoseconds were compared to verify that the transverse resolution and non-square cells were acceptable.

To investigate the dynamics of the plasma ions in a laser wakefield, a high-intensity laser pulse with a Gaussian temporal and transverse spatial envelope

was propagated through a pre-ionised electron-proton plasma. The laser generates a periodic oscillation of the electron density at the plasma frequency, shown in Figure 5.1 during the excitation. The simulation window was fixed, and the laser pulse entered the simulation from the left and exited on the right boundary. All boundaries were absorptive to electromagnetic radiation and reflective to electron and ion particles. The duration and spatial width of

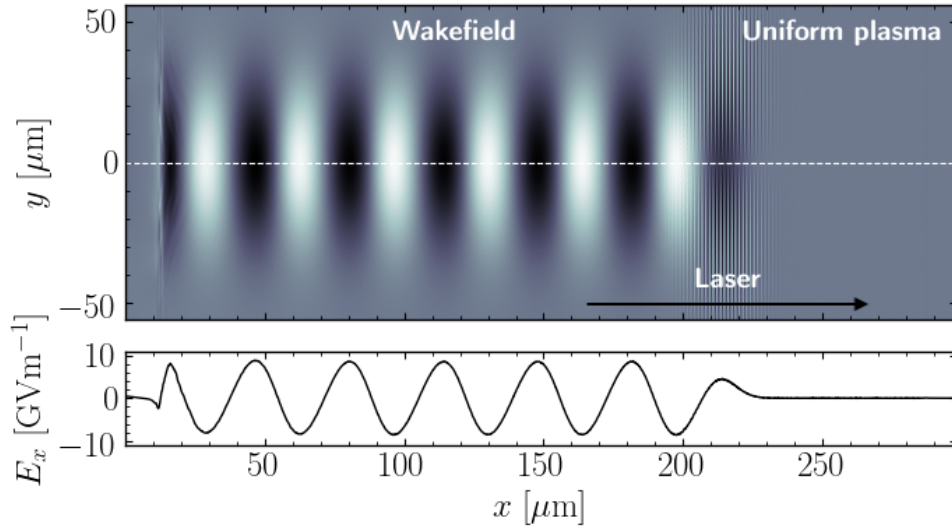


Figure 5.1: *Top*: plot of the longitudinal electric field $E_x(x, y)$ during wakefield excitation. The laser pulse propagates from left to right through a uniform slab of plasma. *Bottom*: line-out of the longitudinal electric field $E_x(x, y = 0)$.

the laser pulse were set to 45 fs (FWHM) and 45 μm (FWHM), respectively. The pulse has a central wavelength of $\lambda_0 = 802.5$ nm and peak intensity $I_{\text{peak}} = 0.53 \times 10^{18} \text{ Wcm}^{-2}$, corresponding to a normalised vector potential, $a_0 = 0.5$. These pulse parameters were selected to generate a wakefield with a density variation amplitude $\delta n_e/n_{e0} \approx 10\%$. In this regime the wakefield energy significantly exceeds the plasma thermal energy, but relativistic effects are weak. The plasma has a longitudinal and transverse extent of 240 μm and 160 μm , respectively, at a uniform plasma density, $n_{e0} = 9.7 \times 10^{17} \text{ cm}^{-3}$.

The plasma dimensions were selected to provide a sufficiently large region unaffected by edge effects, while minimising the size of the simulation domain. The electron temperature was initialized as $T_e = 15 \text{ eV}k_B^{-1}$, near the ionisation energy of hydrogen of $13.6 \text{ eV}k_B^{-1}$. Note that a higher electron temperature alleviates the difficulty of resolving the Debye length of the plasma. The initial ion temperature was set to the gas temperature prior to ionization, $T_i = 0.08 \text{ eV}k_B^{-1}$. The simulation properties and laser and plasma parameters are summarised in Table 5.1.

5.3 DIAGNOSTICS

Several diagnostics were employed to permit a quantitative analysis of the simulations. The three spatial components of the electric and magnetic fields and the electron and ion number densities were recorded at intervals of 30 electron plasma periods, $\tau_{pe} = 2\pi/\omega_{pe}$, over a two-dimensional region of interest extending over the length of the simulation domain and measuring $100 \mu\text{m}$ transversely. The transverse extent of the diagnostic was selected to capture the transverse extent of the wakefield envelope. The temporal resolution was limited to $30 \tau_{pe}$ by the available memory. The diagnostics, therefore, do not resolve the wakefield oscillations temporally since, by the Nyquist-Shannon theorem, this requires a sampling interval of at most $\tau_{pe}/2$. To permit a temporal spectral analysis, a “fast” diagnostic was set up that returns the fields and densities only on-axis ($y = 0$) – thus with low memory footprint – at short intervals of $\tau_{pe}/10$.

5.4 WAKEFIELD EVOLUTION

The wakefield excited by the laser pulse shown in Figure 5.1 attains a maximum longitudinal electric field strength $E_{x,\text{max}} = 8.5 \text{ GVm}^{-1}$ on the axis $y = 0$,

Simulation properties	
<i>Simulation setup:</i>	
Code	smilei v4.3
Infrastructure	ARCHER ¹
Dimensionality	2D
N_{Cores}	3072
Runtime [h]	10
$\Delta x [\lambda_D]$	1
$\Delta y [\lambda_D]$	5
$\Delta t [t_{\text{CFL}}]$	0.95
N_{PPC}	64
$x_{\text{max}} [\lambda_{pe}]$	8
$y_{\text{max}} [\mu m]$	160
<i>Plasma parameters:</i>	
$n_e [\text{cm}^{-3}]$	9.7×10^{17}
$k_B T_e [\text{eV}]$	15.000
$k_B T_i [\text{eV}]$	0.080
$\lambda_D [\text{nm}]$	29.05
$m_i [m_p]$	1
Z_{ion}	1
<i>Laser parameters:</i>	
$I_{\text{peak}} [\text{Wcm}^{-2}]$	0.53×10^{18}
$\lambda_0 [\text{nm}]$	802.5
$w_{\text{fwhm}} [\mu m]$	45.0
$\tau_{\text{fwhm}} [\text{fs}]$	45.0
a_0	0.5

Table 5.1: Properties and parameters of high-resolution 2D PIC simulations.

with a wavelength $\lambda_p = 33.7 \mu m$ and oscillates at the plasma frequency, since $\omega_{k,pe}^2 = \omega_{pe}^2 + 3k^2 v_{th,e}^2 \approx \omega_{pe}^2$ for wavelengths $\lambda = 2\pi/k$ that are long compared to the Debye length of the plasma, $\lambda_D = (\epsilon_0 k_B T_e / n_e e^2)^{1/2} = 29.1 \text{ nm}$. Using the wakefield amplitude and electron temperature of the plasma one can cal-

culate the ratio of the Langmuir energy density to the plasma thermal energy density

$$W = \frac{1}{2} \frac{\epsilon_0 |E|^2}{n_e k_B T_e} \approx 150 \gg 1, \quad (5.7)$$

where we have assumed that $T_i \ll T_e$ so that the ion thermal energy density can be neglected. Since $W \gg 1$ the wakefield energy is much higher than the plasma thermal energy.

The longitudinal electric field of the plasma oscillation is shown in Figure 5.2, $t = 0.32$ ps after the wakefield excitation. From Gauss' law $\partial E_x / \partial x = -e \delta n_e \sin(k_p x - \omega_{pe} t) / \epsilon_0$, with $k_p = \omega_{pe} / c$, it follows that $\max(E_x) = e \delta n_e c / \omega_{pe} / \epsilon_0$; note that for linear wakefields with a Gaussian envelope the contribution of the transverse wakefield is negligible on-axis (cf. Esarey et al., 2009). The maximum on-axis longitudinal electric field strength $E_{x,\max} = 8.5 \text{ GVm}^{-1}$ then suggests a sinusoidal plasma density oscillation of amplitude $\delta n_e / n_e = 0.091$ on-axis, at the background density $n_e = 9.7 \times 10^{17} \text{ cm}^{-3}$, that was confirmed to match the density oscillation observed in the PIC simulation. The transverse profile of the longitudinal electric field envelope matches the laser pulse width $w_{\text{fwhm}} = 45 \text{ } \mu\text{m}$. The laser pulse duration $\tau_{\text{fwhm}} = 45 \text{ fs}$ is short compared to the electron plasma period; $\tau_e = 2\pi\omega_{pe}^{-1} = 112 \text{ fs}$. After excitation of the wakefield, the subsequent evolution of the plasma was observed.

Within two picoseconds of the wakefield excitation, visible modulations of the longitudinal electric field develop, with a characteristic length on-axis ($y = 0$) of $1.3 \text{ } \mu\text{m}$ that is much smaller than the wakefield wavelength, $\lambda_{pe} = 33.7 \text{ } \mu\text{m}$. The modulations are visible in Figure 5.2 at $t = 2.56$ ps after wakefield excitation and are shown magnified in the lower-right inset of the figure. The timescale for the growth of the modulations is on the order of the ion plasma period, $2\pi\omega_{pi}^{-1} \approx 4.8 \text{ ps}$. Figure 5.2 indicates that the wavelength of the modulations decreases with increasing transverse displacement from the axis $y = 0$. It is also apparent that while the modulations have a strong longitudinal

component, they exhibit transverse variations. The modulation of the electric field is accompanied by a modulation of the ion density, shown in the lower panels of Figure 5.2. These observed perturbations of the ion density are phenomenologically consistent with the modulational instability described in Chapter 4.

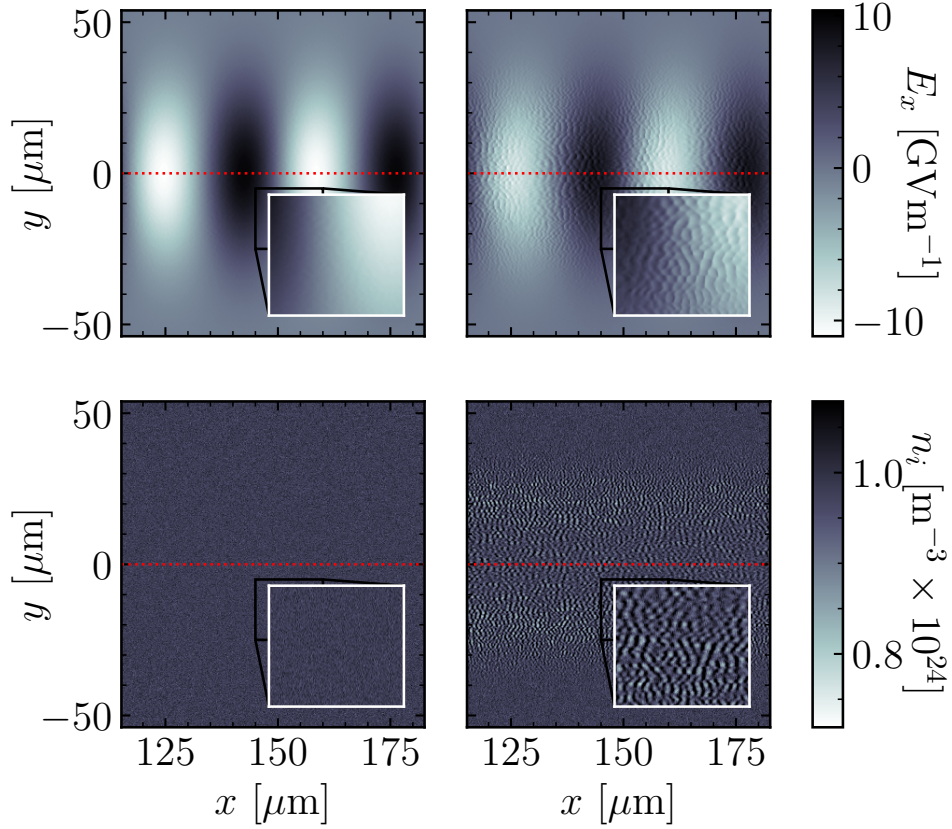


Figure 5.2: *Top row*: longitudinal electric field strength $E_x(x, y)$, $t = 0.32$ ps after wake excitation (*left*) and after $t = 2.56$ ps (*right*), showing the development of high-frequency modulations of the field envelope, magnified in the inset. *Bottom row*: ion density $n_i(x, y)$, showing the development of high-frequency modulations of the ion density. The red line indicates the axis of initial laser propagation.

5.5 COMPARISON WITH THEORY

To investigate the dynamics of the modulations and to perform a comparison with the theory of the strong-field modulational instability (SFMI) reviewed in Chapter 4 a spectral analysis was performed. The longitudinal Fourier transform of the plasma ion density, $\text{FFT}_x[n_i(x, y)]$, was calculated over a region of interest of length $3\lambda_{pe}$, centered in the simulation domain to exclude edge effects. The resulting wave number spectrum is shown in Figure 5.3. The spectrum exhibits an on-axis peak at a wave number $k\lambda_D \approx 0.13$. The wave number of the ion perturbations increases at transverse displacements from the wakefield axis $y = 0$. It is also apparent that the spectra first develop a visible peak at an off-axis displacement $y \approx \pm 20 \mu\text{m}$, indicating that the initial growth rate of the ion density modulation is maximised off-axis. At $t = 3.52$ ps, a second peak, with an on-axis wave number $k\lambda_D \approx 0.27$, has developed that may be a harmonic of the fundamental mode. From the acceleration of an electron in an oscillating electric field it follows that the oscillation speed is given by $v_f \approx \frac{eE_0}{m_e}\omega_{pe}^{-1} = \sqrt{2}W^{1/2}v_{th,e}$, where $v_{th,e} = (k_B T_e/m_e)^{1/2}$ and W measures the ratio of the electric field energy density to the plasma thermal energy density, $W = \epsilon_0 E_0^2 / (n_e k_B T_e)$. Similarly, the displacement of electrons from their equilibrium position is given by $x_f \approx \frac{eE_0}{m_e}\omega_{pe}^{-2} = \sqrt{2}W^{1/2}\lambda_D \gg \lambda_D$. Therefore $v_f \gg v_{th,e}$ and $x_f \gg \lambda_D$. As shown in Chapter 4, this precludes the applicability of the Zakharov equations to describe the modulational instability, since the nonlinear term in the fast timescale electron fluid equation cannot be neglected.

The dispersion relation (4.44) indicates that the instability growth rate is a function of the wave number, electron temperature, electron and ion masses, and the wakefield electric field strength. We numerically solve the Silin-Sanmartin dispersion relation (Sanmartin, 1970) to compare the PIC simulations with theoretical predictions for the modulational instability. To do so,

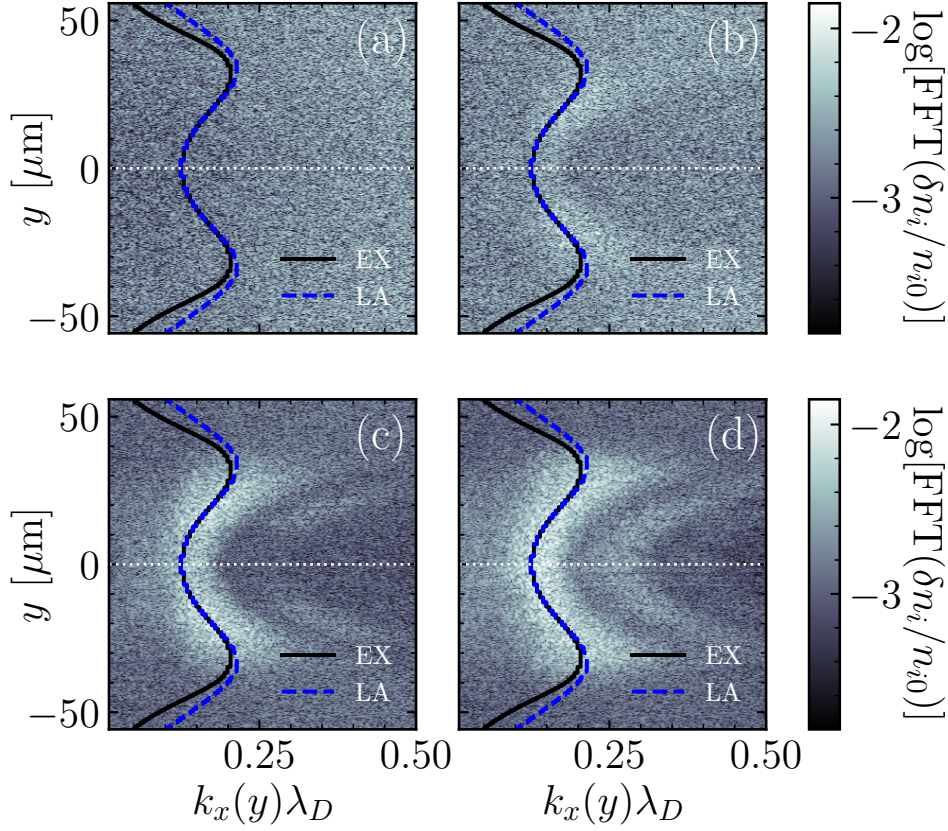


Figure 5.3: Longitudinal wave number spectrum $\text{FFT}_x[n_i(x, y)]$, of the perturbed ion density as a function of transverse position y , at different times after wakefield excitation. (a) $t = 0.64$ ps (b) $t = 1.60$ ps, instability onset off-axis (c) 2.56 ps and (d) $t = 3.52$ ps. The predicted transverse wave number dependence of the fastest growing mode is calculated by solving equation (4.42) (black, solid line) and by solving the approximate equation (4.44) (blue, dashed) valid for a high driving field amplitude near the axis $y = 0$.

equation (4.44) is solved on a wave number grid extending from $k\lambda_D = 0.01$ to $k\lambda_D = 1.0$, by numerically computing the roots of equation (4.44) and selecting the solution, γ , with $\max\{\text{Re}(\gamma) > 0\}$, corresponding to the fastest growing instability. For the quartic equation (4.44) the roots were determined using NumPy's (Harris et al., 2020) root-finding algorithm for polynomials. The quartic dispersion relation is valid for large growth rates $\gamma \gg kv_{th,i}$, expected to be satisfied on-axis but not at large transverse displacements where the wakefield amplitude is low. For comparison, we also solve the dispersion re-

lation given by equation (4.42), which does not rely on the large-amplitude approximation of the plasma dispersion function. We used SciPy's implementation of Brent's root-finding algorithm to solve for the roots of equation (4.42).

5.5.1 FIELD STRENGTH DEPENDENCE

The predicted dependencies of the maximum growth rate and the associated dominant wave number on the wakefield electric field strength are shown in Figure 5.4a and 5.4c, respectively, for the plasma parameters pertaining to the PIC simulations. The growth rate of the modulational instability initially increases with the field strength, is maximised for $E_0 \approx 5.5 \text{ GVm}^{-1}$ and decreases for stronger fields. This non-monotonous growth-rate dependence is associated with the electron displacement in the wakefield oscillations. When the electron excursion distance significantly exceeds the mode wavelength, corresponding to $a \approx ekE_0/(m_e\omega_{pe}^2) \gg 1$ in the Bessel functions in the dispersion relation (4.44), the coupling between the wakefield and the ion perturbations becomes weak as the electrons experience a spatially averaged pondermotive force (Mora et al., 1988); indeed for sufficiently strong fields and large electron displacements the modulational instability is predicted to be suppressed entirely (Sanmartin, 1970). By assuming a transverse Gaussian profile of the wakefield electric field envelope, $E_x(y) = E_0 \exp(-y^2/2\sigma^2)$, with the parameters $E_0 = 8.5 \text{ GVm}^{-1}$ and $\sigma \approx w_{\text{fwhm}} = 45 \text{ }\mu\text{m}$ matched to the values from the PIC simulations, the expected transverse scaling of the dominant wave number can be calculated. To do so, the dispersion relation (4.44) was numerically solved on a transverse grid for the wave number, $k(y)$, that maximises the growth rate. The resulting transverse growth rate and wave number dependence are shown in Figure 5.4b and 5.4d, respectively. At transverse displacements $|y| \lesssim 30 \text{ }\mu\text{m}$, the predicted wave number dependence is in very

good agreement with the transverse variation of the wave number of ion density modulations observed in the PIC simulations, shown in Figure 5.3. At transverse displacements $|y| \gtrsim 30 \mu\text{m}$, the observed wave number continues to increase monotonically with y , whereas the numerical solution of equation (4.44) predicts a decrease in the wave number with greater transverse displacement. This deviation could not be attributed to deviations of the electric field strength from a transverse Gaussian envelope or transverse variations of the plasma density or electron temperature; however, a possible discrepancy may not be significant given the very low signal-to-noise ratio of the measured spectrum near the instability threshold at large transverse displacements.

Figure 5.3b shows that modulations of the ion density first develop at a transverse displacement $y_{\max\{\gamma\}} \sim \pm 20 \mu\text{m}$, indicating that the growth rate is maximised off-axis, where the electric field strength of the wakefield is lower than on-axis. This is consistent with the theoretical scaling of the growth rate with transverse displacements obtained by assuming a transverse Gaussian electric field envelope. Figure 5.4b indicates that for the wakefield amplitude and transverse profile considered here, the maximum growth rate is indeed expected at $y \approx 20 \mu\text{m}$.

5.5.2 ION MASS DEPENDENCE OF THE INSTABILITY GROWTH RATE

To investigate the dependence of the instability growth rate on the ion mass, particle-in-cell simulations were performed for ion masses $m_i = \{0.25, 0.5, 1.0, 2.0, 4.0\}m_p$ with the ion charge and all other simulation parameters held fixed. Growth rates of the ion density perturbations were determined by calculating the longitudinal wave number spectrum on-axis, $\text{FFT}_x[n_i(x, y=0)](k)$, identifying the wave number k_{mod} at which the growth rate is maximised and tracking the amplitude of this mode $A_{k_{\text{mod}}}(t)$ over time

using the fast diagnostic described in Section 5.3. A least-squares linear fit to $\log[A_{k_{\text{mod}}}(t)] = \gamma t + \log A_{k_{\text{mod}}}(t=0)$ was then performed to obtain the growth rate $\gamma(k_{\text{mod}})$. The resulting growth rates are shown as a function of the ion mass in Figure 5.5a and are compared to the predicted mass dependence of the growth rates determined by solving the dispersion relation (4.44). Good agreement between theory and measured growth rates is obtained, confirming that the modulational instability growth rate decreases with increasing ion mass.

5.5.3 TEMPERATURE DEPENDENCE OF THE INSTABILITY GROWTH RATE

The predicted growth rate is shown as a function of the electron temperature in Figure 5.5b (solid black line), obtained by solving equation (4.42) with parameters matched to the default PIC simulation. The dispersion relation predicts a reasonably sharp resonance of the growth rate with electron temperature. Simulations at elevated electron temperatures of $T_e = 100$ eV and $T_e = 1$ keV were performed and growth rates of the ion density perturbations on-axis ($y = 0$) were compared to the theoretical predictions, shown in Figure 5.5b (black squares). Close agreement is obtained at $T_e = 15$ eV; at higher temperatures, the measured growth rates systematically lie below the predicted growth rates, but within 30%, and confirm that at temperatures $T_e \gg 100$ the growth rate of the modulational instability is significantly decreased. It is not clear what causes the systematic discrepancy between measured and predicted growth rates; possible factors are transverse dynamics or a numerical effect related to the resolution of the simulations. For instance, the ratio of the longitudinal and transverse resolution to the Debye length changes for increased electron temperatures, since $\lambda_D \sim T_e^{\frac{1}{2}}$. While for sufficiently hot electrons the modulational instability is suppressed, the three-wave decay of

the equilibrium Langmuir wave into an ion sound wave and second Langmuir wave becomes possible when the required frequency and wave number matching conditions can be satisfied (cf. Sanmartin, 1970; Thornhill and ter Haar, 1978).

5.6 DISCUSSION

The PIC simulations presented here show the development of the strong-field modulational instability in wakefields relevant to multi-pulse laser wakefield accelerators. Measured growth rates and wave numbers and their transverse profiles are in very good agreement with predictions obtained by solving the Silin-Sanmartin dispersion relation for a transverse Gaussian wakefield envelope. The modulational instability develops on a timescale comparable to the inverse ion plasma frequency and will therefore come into play for pulse trains with a duration comparable to the ion plasma period. The non-uniform plasma density associated with the ion density modulations eventually destroys the coherence of electron oscillations in the wakefield, reducing the coupling efficiency between the plasma oscillations and the resonant pulse train (Hooker et al., 2014). Incoherent oscillations may also adversely affect the properties of electron bunches injected for acceleration. Vieira et al. (2012) have investigated the role of ion dynamics in self-modulated proton beam-driven plasma wakefield accelerators. Such accelerators operate in the narrow beam limit (Vieira et al., 2012), where the transverse extent of the proton driver, σ_r , is much smaller than the wavelength of the electron plasma oscillation. In this regime, ion motion is dominated by a strong transverse component since the ponderomotive force of the wakefield envelope scales with the gradient of the wakefield intensity, $F_p \sim \nabla_r E^2 \sim \frac{1}{\sigma_r} E^2$ (Vieira et al., 2012). In contrast, the wakefields investigated here have a transverse scale length set by the laser beam width of $45 \mu\text{m}$ (FWHM) that is greater than the electron plasma

wavelength $\lambda_{pe} = 33.7 \mu\text{m}$. Longitudinal effects are therefore dominant. The small-scale transverse variations observed in Figure 5.2 suggest that transverse effects are non-negligible. Investigating the nature of these variations is beyond the scope of this work but interesting – the perturbed structure is reminiscent of transverse variations in sand ripples on dunes or seabeds.

The results presented here have implications for multi-pulse laser wakefield accelerators. The modulational instability is not expected to significantly affect multi-pulse accelerators driven by pulse trains that are short compared to the growth time scale of the modulational instability. Indeed, simulations performed by the author that are not included here confirmed that a wakefield excited by a pulse train of 20 pulses is unaffected by ion dynamics during the excitation. For pulse trains of a duration that is comparable to or exceeds the ion plasma period, ion dynamics affect the wakefield excitation and ultimately limit the attainable wakefield amplitude (Hooker et al., 2014). The non-monotonic dependence of the SFMI growth rate on the electric field strength, observed transversely in Figure 5.4b, suggests that the per-pulse intensity in long trains can be tuned within trains to minimise the time in which the wakefield amplitude maximizes the SFMI growth-rate. The use of heavy-ion species is a further viable mitigation method if sufficiently high mass-to-charge ratios can be attained. Electron heating, for instance, by a long pre-pulse or by employing a circular polarisation of the driving laser, may also be a viable method to mitigate the effects of ion motion in future multi-pulse laser wakefield accelerators.

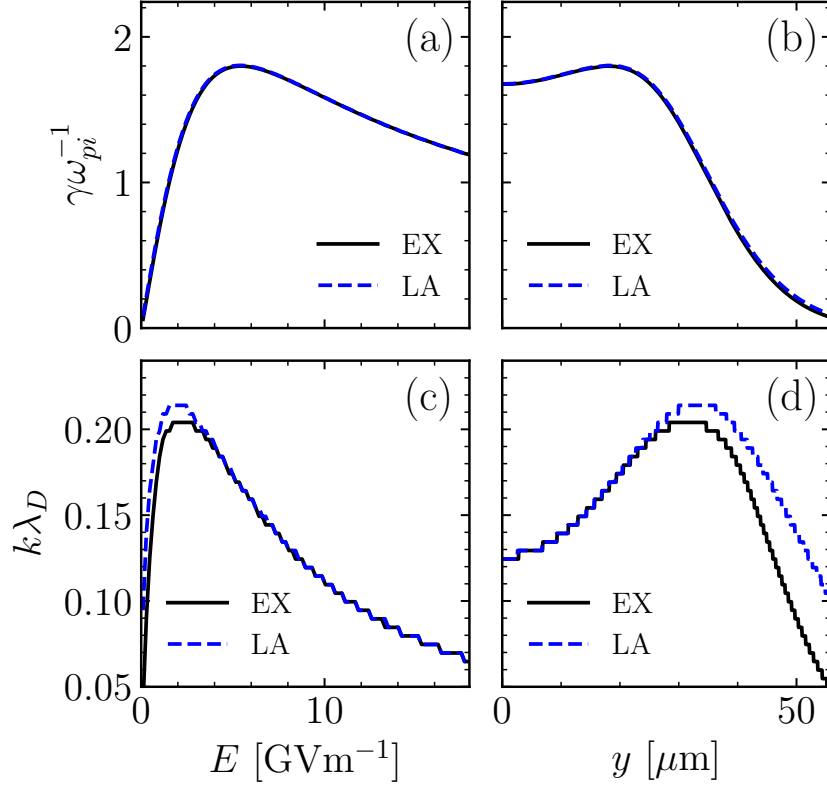


Figure 5.4: Maximum growth rates and dominant wave numbers determined by solving the exact (EX) dispersion relation (4.42) and the large argument (LA) approximation (4.44). (a) maximum growth rate scaling with wake-field electric field strength, (b) transverse dependence of the growth rate for transverse Gaussian wakefield profile, (c) dominant wave number scaling with electric field strength, (d) transverse dependence of the dominant wave number for transverse Gaussian wakefield.

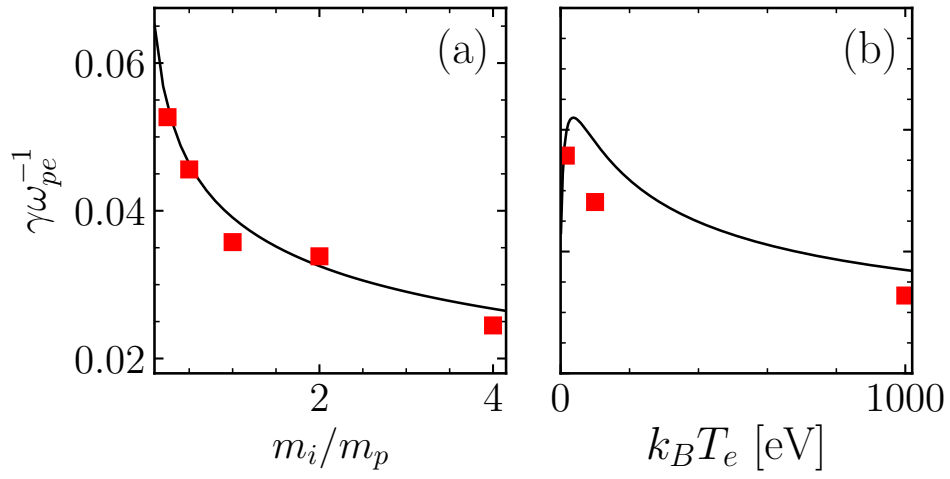


Figure 5.5: (a) Dependence of the modulational instability growth rate on the ion mass (black line), obtained by solving equation (4.42) and measured growth rates from simulations (red squares). (b) Dependence of the growth rate on the electron temperature (black line) and measured growth rates from simulations (red squares).

PART II

A FOKKER-PLANCK COLLISION MODEL FOR GYROKINETIC SIMULATIONS IN STELLARATORS

CHAPTER 6

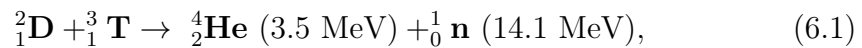
INTRODUCTION

This second part of the thesis introduces a collision model and its implementation for numerical simulations of turbulence in nuclear fusion reactors.

6.1 THERMONUCLEAR FUSION

Reconciling rising global energy demand with reduced emission of greenhouse gases may require novel energy technologies. The nuclear fusion reactor is one proposed energy source that could contribute to a future energy economy. Besides this near-term consideration, there is a fundamental argument for fusion energy – control of such a powerful and abundant energy source will have long-term implications for civilisation by enabling technology that, at this point in time, may not yet be conceivable.

Fusion reactors generate energy by fusing nuclei of light elements, such as hydrogen, into nuclei of heavier elements, such as Helium. The reaction of deuterium nuclei with tritium nuclei



releases a large amount of energy in the form of an alpha particle (3.5 MeV) and a neutron (14.1 MeV). The kinetic energy of the neutron can be converted

into heat by decelerating the neutron in the reactor wall. The resulting thermal energy can then be converted into electricity via a steam cycle.

The reaction (6.1) is mediated by the nuclear strong force that is dominant on distances on the order of the size of nucleons ($\sim 10^{-15}$ m). To trigger the reaction, the positively charged Deuterium and Tritium nuclei must therefore be brought sufficiently close together. This requires work against the long-range repulsive electrostatic force between the charged nuclei. To provide the reactants with sufficient energy to overcome this 'Coulomb barrier', the Deuterium and Tritium species may be heated to high temperatures, on the order of 10 keV. At such temperatures, the electrons and ions dissociate and, together, constitute a plasma – a mixture of ions and free electrons that is characterised by global charge neutrality, high electrical conductivity, and, as a result, collective motion in response to electromagnetic fields.

6.2 MAGNETIC CONFINEMENT

In a thermonuclear fusion reactor, a plasma must be heated to and sustained at temperatures and densities that maximise the number of nuclear reactions. The extreme temperature difference between the hot plasma and ambient surroundings requires exceptional thermal insulation to prevent a rapid cool-down of the plasma species and loss of reactivity. Such insulation can be achieved by exploiting the collective motion of plasmas in response to electromagnetic fields: magnetic fields can be applied to a plasma to confine the motion of charged plasma particles to a region enclosed by the fields, thus preventing contact with the cold surroundings. A plasma confined by a field $\mathbf{B}$ satisfies a balance between a force due to the magnetic pressure $\mathbf{j} \times \mathbf{B}$, where $\mathbf{j}$ is the current density in the plasma, and a force due to the thermal pressure

gradient ∇p :

$$\mathbf{j} \times \mathbf{B} = \nabla p. \quad (6.2)$$

The force balance (6.2) implies that $\mathbf{B} \cdot \nabla p = 0$; that is, magnetic fields are everywhere tangent to surfaces of constant pressure. It is a fundamental property of topology that only a torus permits $\mathbf{B} \cdot \nabla p = 0$ everywhere (Boozer, 2005). The two workhorses in fusion research are thus the *tokamak* and *stellarator* approaches, both of which magnetically confine plasma in a toroidal geometry.

Charged particles in a magnetically confined plasma execute circular motion around magnetic field lines and can stream along field lines. For a purely toroidal magnetic field, the magnetic field strength dependence of the radius of this gyromotion leads to drifts across the field that arise due to the stronger magnetic fields on the inboard side of the torus compared to the outboard side. Helical magnetic fields can be used to stabilise the motion of plasma particles against these drifts by ensuring that particles alternately travel through the strong-field region on the inboard side of the torus and the weak-field region on the outboard side, with drifts in the two regions compensating sufficiently for practicable confinement timescales. In a tokamak, helical fields are generated by combining the toroidal field generated by electromagnetic coils that enclose the plasma poloidally, with a poloidal magnetic field that is created by a solenoidal current through the plasma itself. The solenoidal plasma current is induced by a transformer situated in the center of the torus. Since induction requires a time-varying current in the primary coil of the transformer, tokamaks typically rely on a pulsed operation. The reliance on a plasma current to generate the confining magnetic field is a disadvantage of tokamaks: the current drive can lead to a variety of magneto-hydrodynamic (MHD) instabilities that can inhibit the performance of tokamaks and place operational constraints on such devices.

6.3 STELLARATORS

The stellarator, on the other hand, creates helical magnetic fields via complex shaping of the external magnetic field coils. As a result, no induced plasma current is required, and disruptions due to the current drive in tokamaks cannot occur. The absence of an induced current also permits steady-state operation of stellarators and operation at higher plasma densities (Greenwald, 2002). These advantages of stellarators come at the cost of engineering complexity of the coil systems (but with the benefit of interesting aesthetics) shown in Figure 6.1 for the Wendelstein 7-X stellarator (W7-X), and complicated geometrical effects on particle dynamics in the device: in particular, not all particle trajectories in the magnetic fields of stellarators are confined. Particles that are trapped between two maxima of the magnetic field within one field period drift out of the plasma (Gibson and Taylor, 1967). Such trapped particle populations are prevalent in stellarators due to the complicated magnetic field geometry and lead to high levels of the so-called neoclassical transport (Hinton and Hazeltine, 1976), that can exceed transport due to classical diffusion by orders of magnitude. The magnetic field geometry of modern stellarators, such as W7-X, is carefully optimised computationally in the design of the device to minimise neoclassical losses. Experimental operation of the optimised stellarator W7-X has confirmed that neoclassical transport is indeed successfully reduced (Beidler et al., 2021) to levels that make optimised stellarators a feasible approach to fusion power. While the complexity of the magnetic field coils in stellarators results in engineering challenges, the absence of an externally induced toroidal plasma current lends stellarators to computational design since the magnetic field is predominantly generated by the external coils.

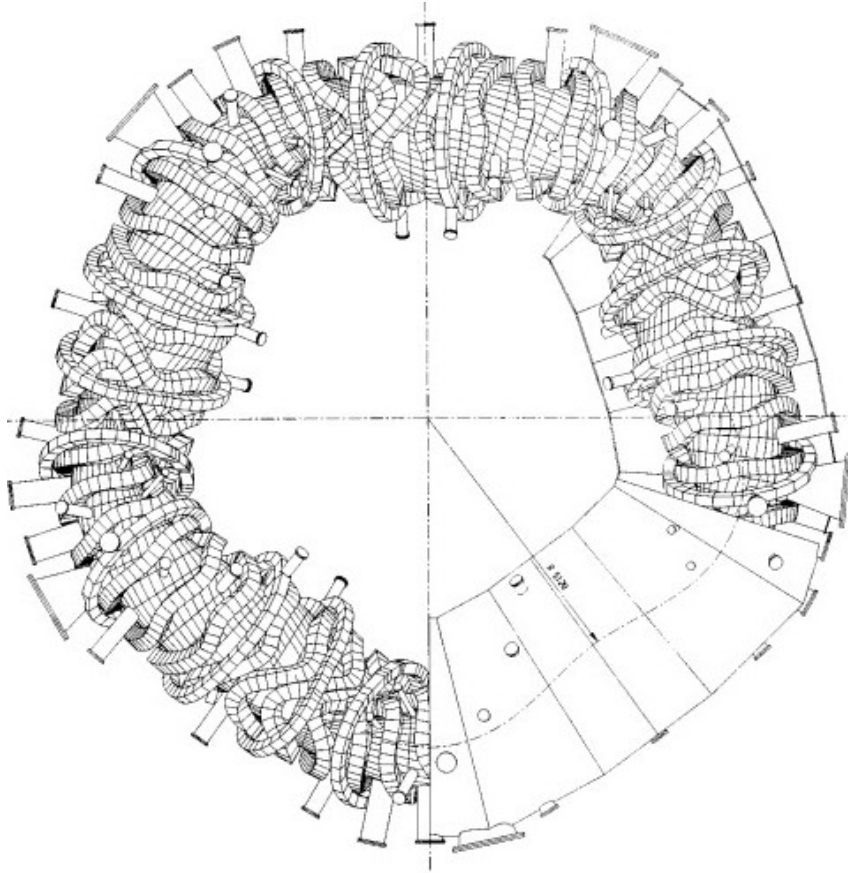


Figure 6.1: Technical drawing of the Wendelstein 7-X coil system by Sapper (1991), showing the non-planar poloidal coils used to generate a helical magnetic field.

6.4 TURBULENCE IN FUSION PLASMAS

It is the objective of magnetic confinement to control the transport of heat and particles out of the plasma – in a self-sustaining fusion burn, the heat lost from the plasma must be compensated by the energy of the alpha particles that sustain the plasma temperature. In magnetic confinement devices, in addition to the gyromotion along magnetic field lines, particles diffuse across the magnetic field due to collisions, with a diffusion step size comparable to the gyroradius. This 'classical' diffusive transport is relatively benign compared to neoclassical and turbulent transport. In tokamak reactors, turbulence is the

dominant transport mechanism. In non-optimized stellarators, neoclassical transport can be significant and can exceed turbulent transport. In stellarators optimised for low neoclassical transport such as W7-X, neoclassical transport is strongly reduced, and turbulence is relatively important: indeed, a comparison of measured heat fluxes in W7-X with calculated neoclassical fluxes suggests a turbulent contribution that is comparable to neoclassical transport levels (Klinger et al., 2019). The turbulent motion of plasma in fusion reactors is driven by gradients in the plasma temperature and density that can lead to instabilities of drift waves. Because the resulting instabilities typically occur on a spatial scale comparable to the ion and electron Larmor radii, they are referred to as microinstabilities to distinguish them from macroscopic phenomena such as MHD instabilities.

The most common microinstabilities include the ion- and electron-temperature gradient driven instabilities (abbreviated ITG and ETG, respectively) and the trapped electron mode (TEM). The former two modes arise due to an unstable growth of plasma waves associated with magnetic, $\mathbf{E} \times \mathbf{B}$ or parallel particle drifts – so-called drift waves – driven by the plasma temperature gradients; the latter arises due to a resonance of trapped electrons with drift waves (cf. Horton, 1999). Experimental observations of density fluctuations in W7-X indicate that ITG microinstabilities develop in the plasma core; this observation is consistent with predictions from numerical simulations (Klinger et al., 2019). On the other hand, TEM instabilities can be mitigated in optimised stellarators if the regions of particle trapping coincide with regions of stabilising magnetic curvature (cf. Helander et al., 2012). Recent gyrokinetic simulations suggest that microinstabilities in stellarators are sensitive to the field configuration of the device (Alcusón et al., 2020), and simulations have been performed that demonstrate the feasibility of turbulent transport-optimised stellarators (Mynick et al., 2010; Xanthopoulos et al., 2014). Linear simulations with the

GENE code (Jenko et al., 2000) have shown that the basic properties of microinstabilities in W7-X are comparable to those in large aspect ratio tokamaks but are affected by the complex geometry of the device (Xanthopoulos and Jenko, 2007). This is consistent with simulations indicating that turbulence can be strongly localized to certain regions in the magnetic field geometry of W7-X (Proll et al., 2013; Cole et al., 2019). Indeed, the effect of the magnetic geometry on turbulent transport and the vast freedom for geometrical optimisation afforded by stellarators compared to axisymmetric devices make stellarators attractive candidates for future reactor designs.

Turbulence in strongly magnetised fusion plasmas has several characteristic properties: the high temperature and low density of particles in fusion plasmas imply that the collision time and the collisional mean free path are large compared to turbulent time and length scales. As a result, the particle dynamics and turbulence cannot be adequately described by fluid models, and one must deal with the complexities of kinetic theory. Critical simplifications are afforded by the strong magnetic field in fusion plasmas that leads to scale separations: the perpendicular scale length of the turbulence, typically on the order of the Larmor radius, is small compared to the scale length of equilibrium density and temperature gradients. As a consequence, the profile gradients can be assumed to be constant when studying the local properties of turbulence. The short perpendicular scale length of the turbulence also implies that the turbulent decorrelation length is small compared to the device size so that statistical periodicity in the perpendicular direction can be assumed, and the turbulence can be investigated in a narrow cylindrical volume around a magnetic field line known as a flux tube. A scale separation also applies to the temporal dynamics of turbulence: the time scale over which turbulent eddies fluctuate, comparable to the drift wave frequency, is fast compared to

the slow evolution of the plasma equilibrium; this permits the simplifying assumption of a static equilibrium when studying the turbulence. On the other hand, the turbulent fluctuation timescale is long compared to the timescale of the fast gyration of particles around magnetic field lines. This time scale separation makes it possible to average over the fast gyromotion of particles. Thus eliminating the gyromotion significantly decreases the complexity of the problem by reducing the dimensionality.

6.5 GYROKINETICS

The temporal and spatial scale separations introduced here underpin the theoretical machinery of *gyrokinetics* that is commonly used to study turbulence in strongly magnetised plasmas. We briefly review the gyrokinetic framework (cf. Catto, 1978; Frieman and Chen, 1982), following the exposition by Howes et al. (2006). If the coupling between plasma particles is weak, the distribution function, f_s , of a particle species, s , in a plasma is described by the Vlasov-Landau equation

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla f_s + \frac{q_s}{m_s} \left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B} \right) \cdot \nabla_{\mathbf{v}} f_s = \sum_{s'} C[f_s, f_{s'}], \quad (6.3)$$

where q_s and m_s denote the species charge and mass respectively, and the sum on the right-hand side accounts for collisions between particles of the species s and between s and particles of other plasma species s' . The terms on the left-hand side in Eq. (6.3) describe, from left to right, the temporal evolution of the distribution function, convection, and acceleration due to the Lorentz force of self-consistent electric and magnetic fields generated by the plasma. The fields $\mathbf{E}$ and $\mathbf{B}$ are mean fields that are calculated via moments of the distribution function to obtain charge and current densities and Maxwell's equations. Due to the strong magnetic field present in magnetic confinement

fusion plasmas we assume throughout this work that the electric field is electrostatic. Collisions in a plasma, described by the collision operator $C[f_s, f_{s'}]$, are predominantly pair-wise, small-angle Coulomb interactions that can be modelled statistically using the Landau-Fokker-Planck operator, described in detail in the subsequent chapter. If collisional effects are included, Eq. (6.3) is then a Fokker-Planck equation.

The kinetic equation (6.3) describes the evolution of the distribution function in time and in the six-dimensional phase space of position and velocity, $(\mathbf{x}, \mathbf{v}) \in \mathbb{R}^6$. The scale separations introduced previously can be used to simplify the problem. The strong magnetisation implies that the Larmor radius ρ_s is small compared to the scale length L of the macroscopic equilibrium:

$$\rho_s = \frac{v_{th,s}}{\Omega_s} \ll L, \quad (6.4)$$

where $\Omega_s = q_s B_0 / (m_s c)$, q_s denotes the species charge, B_0 the magnetic field strength, m_s the species mass and c is the speed of light in vacuum. Eq. (6.4) defines the small parameter $\epsilon := \rho_s / L \ll 1$. The fluctuation frequency of the turbulence ω is taken to be small compared to the cyclotron frequency Ω_s , but it is assumed that turbulent fluctuations take place on timescales that are long compared to the timescale τ , on which the equilibrium profiles of the confined plasma evolve:

$$\frac{1}{\tau} \ll \omega \sim \epsilon \Omega_s \ll \Omega_s. \quad (6.5)$$

One may then split quantities in the kinetic equation into an equilibrium part and a component that fluctuates with the turbulent fluctuations $f_s = F_{0s} + \delta f_s$, $\mathbf{B} = \mathbf{B}_0 + \delta \mathbf{B}$ and $\mathbf{E} = \delta \mathbf{E}$, where we have assumed the absence of a background electric field. The following gyrokinetic ordering is adopted:

$$\frac{\delta f_s}{F_{0s}} \sim \frac{\omega_s}{\Omega_s} \sim \frac{\delta \mathbf{B}}{B} \sim \frac{q\phi}{T} \sim \frac{\rho_s}{L} = \epsilon \ll 1, \quad (6.6)$$

where we have introduced the electrostatic potential ϕ , with $\delta\mathbf{E} = -\nabla\phi$ in the electrostatic limit. The strong magnetisation also implies that perpendicular and parallel gradients of the fluctuating component of the distribution function can be assumed to vary on the scale of the Larmor radius and the equilibrium scale length, respectively:

$$\nabla_{\perp}\delta f_s \sim \frac{\delta f_s}{\rho_s}, \quad \nabla_{\parallel}\delta f_s \sim \frac{\delta f_s}{L}. \quad (6.7)$$

This anisotropy assumption for the turbulence in fusion plasmas is consistent with experimental measurements of the perpendicular and parallel wave number spectra, typically performed by laser or microwave scattering (cf. Liewer, 1985). The collision frequency ν_s is assumed to be comparable to the turbulent fluctuation frequency but small compared to the gyrofrequency

$$\frac{\nu_s}{\Omega_s} \sim \epsilon \ll 1. \quad (6.8)$$

The gyrokinetic ordering thus established can be used to perform an asymptotic expansion of the Vlasov-Landau equation (6.3) in the small parameter ϵ . Expanding the distribution function accordingly

$$f_s = F_{0s} + \delta f_{1s} + \delta f_{2s} + \dots \quad (6.9)$$

with $\delta f_{sN}/F_{0s} \sim O(\epsilon^N)$, one finds, to lowest order in Eq. (6.3), that the equilibrium distribution function is independent of the gyroangle

$$\frac{\partial F_{0s}}{\partial \varphi} = 0. \quad (6.10)$$

Retaining terms up to $O(\epsilon^0)$ in Eq. (6.3), the equilibrium distribution function is uniquely constrained by the collision operator to be Maxwellian (cf. Howes et al., 2006)

$$F_{0s}(v) = \frac{n_{0s}}{\pi^{3/2} v_{th,s}^3} \exp\left(-\frac{v^2}{v_{th}^2}\right). \quad (6.11)$$

Using this property in the zeroth order equation and performing a spatial average to eliminate fluctuating quantities, the solution of the zeroth order gyrokinetic equation is given by

$$f_s = F_{0s} - \underbrace{\frac{q_s \phi}{T_0} F_{0s} + h_s(\mathbf{R}, v_\perp, v_\parallel)}_{:= \delta f_{1s}} + \delta f_{2s} + \dots, \quad (6.12)$$

where the second term on the right-hand side describes the Boltzmann response of the particles to the electrostatic potential. The function $h(\mathbf{R}, v_\perp, v_\parallel) := \delta f_{s1} + q_s \phi F_{0s}/T_{0s}$ is the non-Boltzmann component of the first order perturbation δf_{s1} and is independent of the gyroangle when expressed in coordinates of the particle guiding center $\mathbf{R} := \mathbf{r} - \boldsymbol{\rho}$, where $\boldsymbol{\rho} = \hat{\mathbf{b}} \times \mathbf{v}/\Omega_s$ denotes the gyrovector; h_s can thus be interpreted as a distribution function of charged rings (cf. Howes et al., 2006).

The temporal scale separation implies that δf_2 is periodic in the gyroangle. This motivates the gyroaverage, to eliminate δf_2 , given by

$$\langle \cdot \rangle_{\mathbf{R}} = \frac{1}{2\pi} \int_0^{2\pi} \cdot d\varphi, \quad (6.13)$$

and performed while holding the guiding center, $\mathbf{R}$, fixed. Substituting the zeroth order solution (6.12) in the Vlasov-Landau equation and retaining terms up to first order one obtains an equation for h that includes δf_2 . Eliminating the δf_2 term by transforming into gyrocenter coordinates $\mathbf{r} \rightarrow \mathbf{R} = \mathbf{r} - \boldsymbol{\rho}$ and performing the gyroaverage, one obtains the electrostatic gyrokinetic equation for the distribution function h

$$\begin{aligned} \frac{\partial h}{\partial t} + (v_\parallel \hat{\mathbf{b}} + \mathbf{v}_D + \langle \mathbf{v}_E \rangle_{\mathbf{R}}) \cdot \nabla h - \frac{\mu}{m} \hat{\mathbf{b}} \cdot \nabla \mathbf{B} \frac{\partial h}{\partial v_\parallel} \\ + \left(\langle \mathbf{v}_E \rangle_{\mathbf{R}} \cdot \nabla - \frac{q}{T} \frac{\partial \langle \phi \rangle}{\partial t} \right) F_0 = \langle C[h] \rangle_{\mathbf{R}}. \end{aligned} \quad (6.14)$$

where we have suppressed species indices. Note that Eq. (6.14) is written in terms of the distribution function h ; switching to $\delta f_1 = h(\mathbf{R}, v_\perp, v_\parallel) - q\phi F_0/T_0$

makes the electric field explicit in the gyrokinetic equation via $\mathbf{E} = -\nabla\phi$ in the electrostatic limit, where the inductive field $-d\mathbf{A}/dt$ was ordered to be small. The gyrokinetic equation describes the dynamics of a distribution function of charged rings, obtained by averaging over the fast Larmor gyration of the particles around the magnetic field lines. From left to right, in the top line, the terms in the gyrokinetic equation describe the temporal evolution, advection in the form of parallel streaming and due to magnetic ($\mathbf{v}_D$) and $\mathbf{E} \times \mathbf{B}$ drifts ($\mathbf{v}_E$), and parallel acceleration. In the lower line, the left-hand side terms account for advection of the equilibrium due to the turbulent $\mathbf{E} \times \mathbf{B}$ drift, and work done by the electric field on the charged rings (Howes et al., 2006). The right-hand side describes the action of collisions between particles on the distribution function. The magnetic drift velocity, due to gradient and curvature drifts is given by

$$\mathbf{v}_D = \frac{\hat{\mathbf{b}}}{\Omega} \times \left(\frac{v_\perp^2}{2} \frac{\nabla \mathbf{B}}{B} + v_\parallel^2 \hat{\mathbf{b}} \cdot \nabla \hat{\mathbf{b}} \right), \quad (6.15)$$

and the turbulent $\mathbf{E} \times \mathbf{B}$ -drift velocity is given by

$$\mathbf{v}_E = \frac{c}{B} \hat{\mathbf{b}} \times \nabla_\perp \phi, \quad (6.16)$$

where ϕ denotes the fluctuating electrostatic potential.

6.6 GYROKINETIC SIMULATIONS AND THE CODE `stella`

The gyrokinetic equation can be solved analytically in some special cases but in general requires a numerical approach. Compared to tokamaks, few numerical studies of turbulence have been performed for stellarators, and with relatively few exceptions (eg. Kauffmann et al., 2010; Sánchez et al., 2019; Alcusón et al., 2020, not exhaustive), the gyrokinetic simulations in stellarators performed to date have been collisionless. However, it is well known that

collisions play a fundamental role in gyrokinetics as a dissipation mechanism, even in weakly collisional plasmas (Abel et al., 2008; Barnes et al., 2009) because the presence of a dissipation term is required for steady-state simulations of turbulence. Collisions can also be important in highly collisional edge regions of the plasma, as a detrapping mechanism for particles caught in magnetic wells (Alcusón et al., 2020) or for highly charged ion species, since the collision frequency scales with the fourth power of the species charge. The transport of impurity ions is particularly important in magnetically confined plasmas because the accumulation of impurities in the plasma core leads to radiative energy loss via line radiation and Bremsstrahlung; in both cases, the power radiated increases with the impurity charge. These considerations motivate collisional gyrokinetic simulations of stellarators.

The gyrokinetic code `stella` solves the gyrokinetic equation (6.14) in a general magnetic geometry, thus permitting simulations in the non-axisymmetric geometries of stellarators. The code advances the gyrokinetic equation in terms of the guiding center distribution function $g := \langle \delta f_1 \rangle = \langle h - q\phi F_0/T_0 \rangle = h - q\langle \phi \rangle F_0/T_0$. The spatial coordinates perpendicular to the magnetic field, x and y , are treated spectrally by decomposing the distribution function into Fourier harmonics. This ensures periodicity in the perpendicular coordinates, an acceptable assumption because turbulence is statistically periodic over spatial scales that are short compared to the device size. The field-line parallel coordinate z is discretised on a uniform grid. The code uses $(v_{\parallel}, \mu)$ -velocity space coordinates, where $v_{\parallel}$ is the velocity component parallel to the magnetic field, and $\mu = mv_{\perp}^2/2B_0$ denotes the magnetic moment. The velocity grid is described in some detail in the following chapter. Uniquely, `stella` makes use of an operator splitting method to separate the fast parallel streaming and acceleration from the slower perpendicular dynamics in the numerical treatment. The former can then be treated implicitly to ameliorate the CFL

timestep constraint otherwise associated with an explicit treatment of the parallel dynamics. A detailed description of `stella` is given in Barnes et al. (2018).

To date `stella` used a collision model that is a relatively crude approximation of the Fokker-Planck collision operator obtained by assuming collision frequencies that are independent of the particle speed (Dougherty, 1964) and neglecting interspecies collisions. In the following chapters, we describe a novel collision model for numerical simulations of stellarator turbulence and its implementation in `stella`. The collision model combines an exact treatment of the diffusive component of the Fokker-Planck operator with a series approximation of the drag component of the operator that is based on an expansion developed by Hirshman and Sigmar (1976). Interspecies collisions are included for an arbitrary number of species. The collision operator thus obtained and implemented in `stella` constitutes the first implementation of a collision model with scalable accuracy in a gyrokinetic code.

CHAPTER 7

THEORY OF THE COLLISION MODEL

7.1 COLLISIONS

The effect of pair-wise small-angle Coulomb collisions between distribution functions of two species f_a and f_b is described by the Landau-Fokker-Planck operator (Landau, 1936, cf. Helander and Sigmar (2002))

$$C_{ab}[f_a, f_b] = \frac{\partial}{\partial v_k} \left[A_k^{ab} f_a + \frac{\partial}{\partial v_l} (D_{kl}^{ab} f_a) \right], \quad (7.1)$$

where the Einstein summation convention is used and the tensors A_k^{ab} and D_{kl}^{ab} are given by

$$\begin{aligned} A_k^{ab} &:= L^{ab} [1 + m_a/m_b] \frac{\partial}{\partial v_k} \underbrace{\int \frac{f_b(\mathbf{v}')}{u} d^3 v'}_{=: \phi_b(\mathbf{v})} \\ D_{kl}^{ab} &:= -L^{ab} \frac{\partial^2}{\partial v_k \partial v_l} \underbrace{\int u f_b(\mathbf{v}') d^3 v'}_{=: \psi_b(\mathbf{v})}, \end{aligned} \quad (7.2)$$

with $u := |\mathbf{v} - \mathbf{v}'|$ and $L^{ab} = (e_a e_b / m_a \epsilon_0)^2 \ln \Lambda$, where $\ln \Lambda$ is the Coulomb logarithm. We have also defined the Rosenbluth potentials $\phi_b(\mathbf{v})$ and $\psi_b(\mathbf{v})$. It can be shown that the collision operator given by Eq. (7.1) conserves particle number, momentum and energy. The operator is also self-adjoint and as a result satisfies an H-theorem, that is, collisions cannot decrease the total

entropy of the plasma. Because the amplitude of plasma fluctuations in the reactor core is typically much smaller than the equilibrium, the distribution function can be split into an equilibrium component and a fluctuating component viz. $f = F_0 + \delta f$, with Maxwellian F_0 and $\delta f/F_0 = \epsilon \ll 1$. Then, to first order

$$\begin{aligned} C^{ab}[f_a, f_b] = & C^{ab}[F_{0a}, F_{0b}] + C_{\text{test}}^{ab}[\delta f_a, F_{0b}] \\ & + C_{\text{field}}^{ab}[F_{0a}, \delta f_b] + O(\epsilon^2). \end{aligned} \quad (7.3)$$

The zeroth-order term describes the collisional temperature equilibration between species and vanishes for $T_a = T_b$. For $T_a \neq T_b$ the term enters into the transport equations that describe the evolution of the equilibrium; subtracting the average of the transport equation over space-time scales that are long compared to the turbulent length scale but short compared to the variations of the equilibrium eliminates the zeroth-order term from the gyrokinetic equation. The first, first-order, 'test-particle' term describes collisions of particles in the perturbed distribution function of species a , with the Maxwellian background of species b ; the second, 'field-particle' term describes collisions of the background particles of species b with the perturbed particles of species a . The two operators have manifestly different structures; their derivations, conversions to gyrokinetic form and numerical implementations are described separately in what follows.

7.2 TEST PARTICLE OPERATOR

The Rosenbluth potentials $\phi_b(\mathbf{v})$ and $\psi_b(\mathbf{v})$ simplify considerably for Maxwellian distribution functions that are isotropic in velocity space. The

test-particle operator can then be written as

$$C_{\text{test}}^{ab}[\delta f_a, F_{0b}] = L^{ab} \frac{\partial}{\partial v_k} \left[\frac{v_k}{v} \phi'_{0b} \delta f_a - \left(\frac{[v^2 \delta_{kl} - v_k v_l]}{v^3} \psi'_{0b} + \frac{v_k v_l}{v^2} \psi''_{0b} \right) \frac{\partial \delta f_a}{\partial v_l} \right], \quad (7.4)$$

where primes denote derivatives with respect to the velocity magnitude, v , and the subscript '0b' indicates Rosenbluth potentials of Maxwellian distribution functions for species b . Replacing the Einstein summation convention with vector products one obtains

$$C_{ab}(\delta f_a, F_{0b}) = L^{ab} \nabla_{\mathbf{v}} \cdot \left[\mathbf{v} \left(\frac{\psi'_{0b}}{v^3} - \frac{\psi''_{0b}}{v^2} \right) \mathbf{v} \cdot \nabla_{\mathbf{v}} \delta f_a + \frac{\mathbf{v}}{v} \phi'_{0b} \delta f_a - \frac{\psi'_{0b}}{v} \nabla_{\mathbf{v}} \delta f_a \right] \quad (7.5)$$

In spherical coordinates, (v, θ, ϕ) , where θ and ϕ denote the pitch- and gyro-angles respectively, we have

$$\nabla_{\mathbf{v}} \cdot \mathbf{A} = \frac{1}{v^2} \frac{\partial(v^2 A_v)}{\partial v} + \frac{1}{v \sin \theta} \frac{\partial(A_\theta \sin \theta)}{\partial \theta} + \frac{1}{v \sin \theta} \frac{\partial A_\phi}{\partial \phi}, \quad (7.6)$$

and

$$\nabla_{\mathbf{v}} f = \frac{\partial f}{\partial v} \hat{\mathbf{v}} + \frac{1}{v} \frac{\partial f}{\partial \theta} \hat{\boldsymbol{\theta}} + \frac{1}{v \sin \theta} \frac{\partial f}{\partial \phi} \hat{\boldsymbol{\phi}} \quad (7.7)$$

where $A_v = \mathbf{A} \cdot \hat{\mathbf{v}}$, for the radial unit vector $\hat{\mathbf{v}}$, and analogously for the remaining components. The test-particle operator is then given by

$$\begin{aligned} C_{ab}[\delta f_a, F_{0b}] &= L^{ab} \left[\frac{1}{v^2} \frac{\partial}{\partial v} \left(v^3 [\psi'_{0b}/v^3 - \psi''_{0b}/v^2] v \frac{\partial \delta f_a}{\partial v} + v^2 \phi'_{0b} \delta f_a - v \psi'_{0b} \frac{\partial \delta f_a}{\partial v} \right) \right. \\ &\quad \left. - \frac{1}{v \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\psi'_{0b}}{v^2} \frac{\partial \delta f_a}{\partial \theta} \right) - \frac{1}{v \sin \theta} \frac{\partial}{\partial \phi} \left(\frac{\psi'_{0b}}{v^2 \sin \theta} \frac{\partial \delta f_a}{\partial \phi} \right) \right] \\ &= L^{ab} \left[\frac{1}{v^2} \frac{\partial}{\partial v} \left(v^2 \phi'_{0b} \delta f_a - v^2 \psi''_{0b} \frac{\partial \delta f_a}{\partial v} \right) - \frac{\psi'_{0b}}{v^3} \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial \delta f_a}{\partial \theta} \right. \\ &\quad \left. - \frac{\psi'_{0b}}{v^3} \frac{1}{\sin^2 \theta} \frac{\partial^2 \delta f_a}{\partial \phi^2} \right]. \end{aligned} \quad (7.8)$$

With $\xi = \cos \theta$ one obtains

$$\begin{aligned}
C_{ab}[\delta f_a, F_{0b}] &= \frac{1}{2} \nu_D^{ab} \frac{\partial}{\partial \xi} (1 - \xi^2) \frac{\partial \delta f_a}{\partial \xi} + \frac{1}{2} \nu_D^{ab} \frac{1}{1 - \xi^2} \frac{\partial^2 \delta f_a}{\partial \phi^2} \\
&\quad + \frac{1}{v^2} \frac{\partial}{\partial v} \left[\frac{1}{2} v^3 \nu_s^{ab} \delta f_a + \frac{1}{2} v^4 v \nu_{\parallel}^{ab} \frac{\partial \delta f_a}{\partial v} \right] \\
&= \frac{1}{2} \nu_D^{ab} \frac{\partial}{\partial \xi} (1 - \xi^2) \frac{\partial \delta f_a}{\partial \xi} + \frac{1}{2} \nu_D^{ab} \frac{1}{1 - \xi^2} \frac{\partial^2 \delta f_a}{\partial \phi^2} \\
&\quad + \frac{1}{v^2} \frac{\partial}{\partial v} \left[\frac{1}{2} \nu_{\parallel}^{ab} v^4 F_{0a} \frac{\partial \delta f_a}{\partial v} F_{0a} \right]. \tag{7.9}
\end{aligned}$$

We have introduced the velocity-dependent collision frequencies (Helander and Sigmar, 2002)

$$\nu_D^{ab} := -2L^{ab} \frac{\psi'_{0b}}{v^3} = \frac{n_b q_a^2 q_b^2 \ln \Lambda}{4\pi m_a^2 \epsilon_0^2 v_{th,a}^3} \frac{\text{erf}(x_b) - G(x_b)}{x_a^3} = \nu^{ab} \frac{\text{erf}(x_b) - G(x_b)}{x_a^3}, \tag{7.10}$$

$$\nu_s^{ab} := 2L^{ab} \frac{\phi'_{0b}}{v} = 2L^{ab} \frac{m_a n_b}{4\pi T_b v_{th}} \frac{G(x_b)}{x_a} = \nu^{ab} \frac{4G(x_b)}{x_a} \tag{7.11}$$

$$\nu_{\parallel}^{ab} := -2L^{ab} \frac{\psi''_{0b}}{v^2} = \nu^{ab} \frac{2G(x_b)}{x_a^3} = \frac{1}{2} \frac{\nu_s^{ab}}{x_a^2} \tag{7.12}$$

where $x_s = v/v_{th,s}$ with $s \in \{a, b\}$ and the Chandrasekhar function is given by $G(x_b) := [\text{erf}(x_b) - x \text{erf}'(x_b)]/2x_b^2$. The basic Spitzer collision frequency ν^{ab} is

$$\nu^{ab} = \frac{n_b e_a^2 e_b^2 \ln \Lambda}{4\pi \epsilon_0^2 m_a^2 v_{th,a}^3}. \tag{7.13}$$

Usefully, in spherical coordinates the diffusive test particle operator separates into three independent components in the three velocity-space variables. The first term in (7.9) describes diffusion in the pitch-angle due to collisions, the second and third terms describe diffusion in the gyro-angle and energy, respectively.

To transform into the $(v_{\parallel}, \mu, \phi)$ -coordinate system employed in **stella**, we use that in Cartesian coordinates $\hat{v} = \sin \theta \cos \phi \hat{x} + \sin \theta \sin \phi \hat{y} + \cos \theta \hat{z}$, and $\hat{\theta} = \cos \theta \cos \phi \hat{x} + \cos \theta \sin \phi \hat{y} - \sin \theta \hat{z}$, whence, by identifying $\hat{z}$ with $\hat{v}_{\parallel}$, $\hat{v}_{\perp} = \cos \phi \hat{x} + \sin \phi \hat{y}$. Here θ denotes the angle between $\vec{v}$ and the z -axis that is

taken to be tangent to the magnetic field, and ϕ denotes the angle between the projection of $\vec{v}$ onto the (x, y) -plane, and the positive x -axis. Then

$$\mathbf{v} = \begin{pmatrix} v_{\perp} \cos \phi \\ v_{\perp} \sin \phi \\ v_{\parallel} \end{pmatrix} = \begin{pmatrix} \sqrt{2B\mu/m} \cos \phi \\ \sqrt{2B\mu/m} \sin \phi \\ v_{\parallel} \end{pmatrix}. \quad (7.14)$$

The new unit vectors are given by $\hat{v}_{\parallel} = \hat{v} \cos \theta - \hat{\theta} \sin \theta$ and $\hat{v}_{\perp} = \hat{v} \sin \theta + \hat{\theta} \cos \theta$. The divergence of a vector $\mathbf{A}$ in a general 3-dimensional curvilinear orthogonal coordinate system is given by

$$\nabla \cdot \mathbf{A} = \frac{1}{h_u h_v h_w} \left[\frac{\partial(A_u h_v h_w)}{\partial u} + \frac{\partial(A_v h_u h_w)}{\partial v} + \frac{\partial(A_w h_u h_v)}{\partial w} \right] \quad (7.15)$$

where $h_u = |\partial \mathbf{r} / \partial u|$, and the analogous expressions hold for h_v and h_w . Then, in $(v_{\parallel}, \mu, \phi)$ -coordinates

$$\begin{aligned} \nabla_v \cdot \mathbf{A} &= \frac{m}{B} \left[\frac{\partial(B/m A_{v_{\parallel}})}{\partial v_{\parallel}} + \frac{\partial(\sqrt{2B\mu/m} A_{\mu})}{\partial \mu} + \frac{\partial(\sqrt{B/2m\mu} A_{\phi})}{\partial \phi} \right] \\ &= \frac{\partial A_{v_{\parallel}}}{\partial v_{\parallel}} + \sqrt{2m/B} \frac{\partial \sqrt{\mu} A_{\mu}}{\partial \mu} + \sqrt{m/2B\mu} \frac{\partial A_{\phi}}{\partial \phi}. \end{aligned} \quad (7.16)$$

and

$$\nabla_v f = \frac{\partial f}{\partial v_{\parallel}} \hat{v}_{\parallel} + \sqrt{2m/B_0} \frac{\partial \sqrt{\mu} f}{\partial \mu} \hat{v}_{\perp} + \frac{1}{\sqrt{2B_0\mu/m}} \frac{\partial f}{\partial \phi} \hat{\phi}. \quad (7.17)$$

For the Laplace operator

$$\Delta A = \frac{1}{h_u h_v h_w} \left[\frac{\partial}{\partial u} \left(\frac{h_v h_w}{h_u} \frac{\partial A}{\partial u} \right) + \frac{\partial}{\partial v} \left(\frac{h_u h_w}{h_v} \frac{\partial A}{\partial v} \right) + \frac{\partial}{\partial w} \left(\frac{h_v h_u}{h_w} \frac{\partial A}{\partial w} \right) \right], \quad (7.18)$$

and thus

$$\Delta_v A = \frac{\partial^2 A}{\partial v_{\parallel}^2} + \frac{2m}{B} \frac{\partial}{\partial \mu} \left(\mu \frac{\partial A}{\partial \mu} \right) + \frac{m}{2B\mu} \frac{\partial^2 A}{\partial \phi^2}. \quad (7.19)$$

The test-particle component of the linearized Fokker-Planck operator then

becomes

$$\begin{aligned}
C_{ab}(\delta f_a, F_{0b}) &= L^{ab} \left[\frac{\partial}{\partial v_{\parallel}} \left(v_{\parallel} [\psi'_{0b}/v^3 - \psi''_{0b}/v^2] \mathbf{v} \cdot \nabla_v \delta f_a + \frac{v_{\parallel}}{v} \phi'_{0b} \delta f_a - \frac{\psi'_{0b}}{v} \frac{\partial \delta f_a}{\partial v_{\parallel}} \right) \right. \\
&\quad + 2 \frac{\partial}{\partial \mu} \left(\mu [\psi'_{0b}/v^3 - \psi''_{0b}/v^2] \mathbf{v} \cdot \nabla_v \delta f_a + \frac{\mu}{v} \phi'_{0b} \delta f_a - \mu \frac{\psi'_{0b}}{v} \frac{m_a}{B_0} \frac{\partial \delta f_a}{\partial \mu} \right) \\
&\quad \left. - \frac{m_a}{2B_0\mu} \frac{\psi'_{0b}}{v} \frac{\partial^2 \delta f_a}{\partial \phi^2} \right] \\
&= \frac{1}{2} \frac{\partial}{\partial v_{\parallel}} \left([\nu_{\parallel}^{ab} v_{\parallel}^2 + \nu_D^{ab} 2B_0\mu/m_a] \frac{\partial \delta f_a}{\partial v_{\parallel}} + 2\nu_x^{ab} \mu v_{\parallel} \frac{\partial \delta f_a}{\partial \mu} + \nu_s^{ab} v_{\parallel} \delta f_a \right) \\
&\quad + \frac{\partial}{\partial \mu} \left([2\mu^2 \nu_{\parallel}^{ab} + \nu_D^{ab} \mu m_a v_{\parallel}^2/B_0] \frac{\partial \delta f_a}{\partial \mu} + \nu_x^{ab} \mu v_{\parallel} \frac{\partial \delta f_a}{\partial v_{\parallel}} + \nu_s^{ab} \mu \delta f_a \right) \\
&\quad + \frac{\nu_D^{ab}}{2} \left(1 + \frac{m_a v_{\parallel}^2}{2B_0\mu} \right) \frac{\partial^2 \delta f_a}{\partial \phi^2}, \tag{7.20}
\end{aligned}$$

where we used that $v_{\perp} = \sqrt{2B_0\mu/m}$, $\mathbf{v} = v_{\parallel} \hat{\mathbf{v}}_{\parallel} + v_{\perp} \hat{\mathbf{v}}_{\perp}$ and defined $\nu_x^{ab} := \nu_{\parallel}^{ab} - \nu_D^{ab}$. The collision operator may be written more compactly as

$$\begin{aligned}
C_{\text{test}}^{ab}[\delta f_a, F_{0b}] &= \frac{\partial}{\partial v_{\parallel}} \left[\gamma_{v_{\parallel}}^{ab} F_{0a} \frac{\partial}{\partial v_{\parallel}} \frac{\delta f_a}{F_{0a}} + v_{\parallel} \mu \nu_x^{ab} F_{0a} \frac{\partial}{\partial \mu} \frac{\delta f_a}{F_{0a}} \right] \\
&\quad + \frac{\partial}{\partial \mu} \left[\gamma_{\mu}^{ab} F_{0a} \frac{\partial}{\partial \mu} \frac{\delta f_a}{F_{0a}} + v_{\parallel} \mu \nu_x^{ab} F_{0a} \frac{\partial}{\partial v_{\parallel}} \frac{\delta f_a}{F_{0a}} \right] \\
&\quad + \frac{\nu_D^{ab}}{2} \left[1 + \frac{v_{\parallel}^2}{2B_0\mu} \right] \frac{\partial \delta f_a^2}{\partial \phi^2}, \tag{7.21}
\end{aligned}$$

where derivatives now act on $\delta f_a/F_{0a}$, which we will see has advantages for the numerical implementation. For compactness we have defined

$$\gamma_{\mu}^{ab} = 2 \left[\nu_{\parallel}^{ab} \mu^2 + \nu_D^{ab} \frac{m_a v_{\parallel}^2}{2B_0} \mu \right], \quad \gamma_{v_{\parallel}}^{ab} = \frac{1}{2} \left[\nu_{\parallel}^{ab} v_{\parallel}^2 + \nu_D^{ab} \frac{2B_0\mu}{m_a} \right]. \tag{7.22}$$

Switching from $\{v, \xi\}$ -coordinates to the parallel velocity and magnetic moment has introduced mixed-differential terms in the collision operator. The collision frequency coefficients occurring in the test particle operator (7.21) are shown in Figures 7.1 and 7.2. Terms occurring in the $v_{\parallel}$ -derivative operator vanish at $v_{\parallel} \rightarrow \pm\infty$; terms in the μ -derivative operator vanish for $\mu \rightarrow 0$ and $\mu \rightarrow \infty$. These asymptotics will be relevant for the numerical implementation of the collision operator.

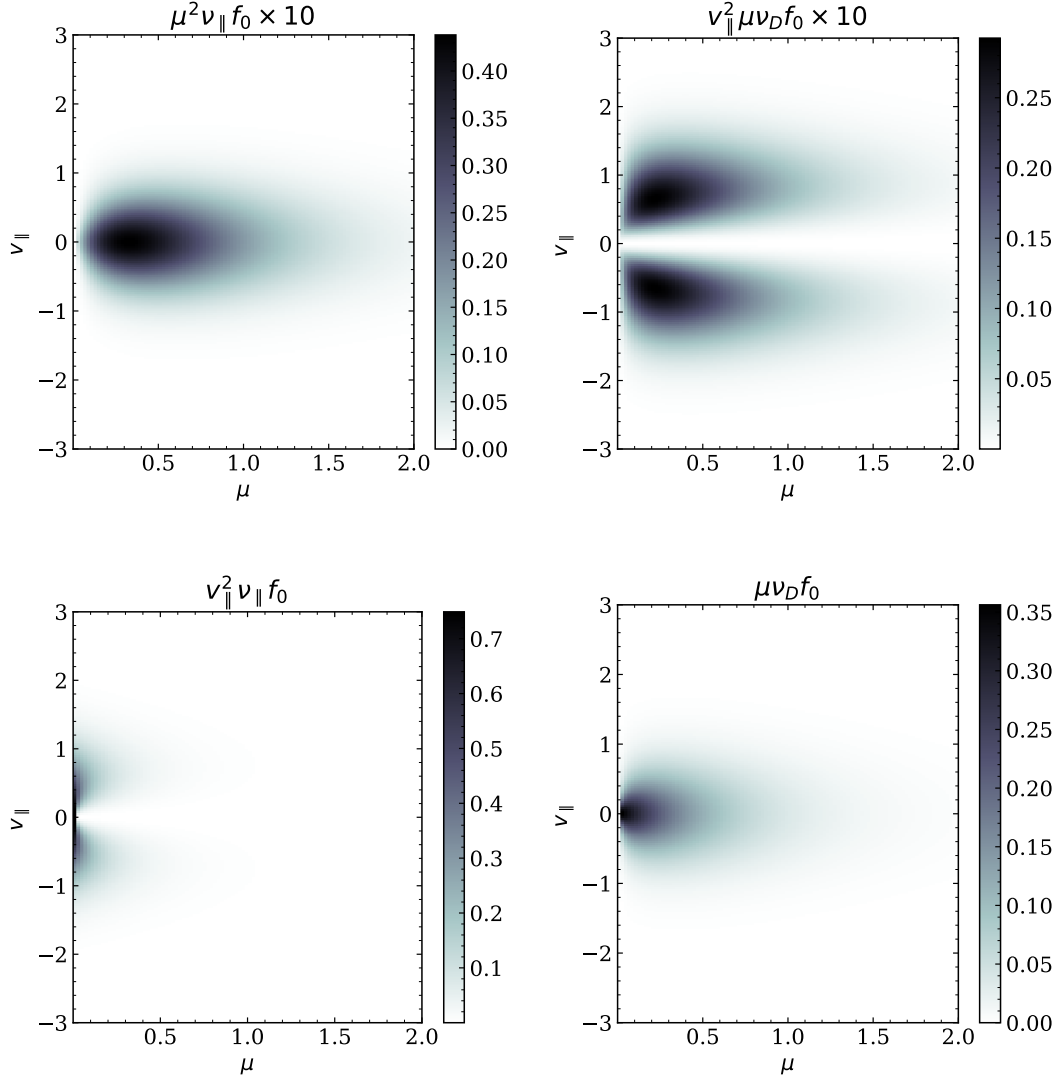


Figure 7.1: Collision frequency terms occurring in the test particle operator (7.21), for like-species collisions. *Top row:* terms occurring in the μ -differential term, vanishing for $\mu \rightarrow 0$ and $\mu \rightarrow \infty$. *Bottom row:* terms in the $v_{\parallel}$ -derivative term, vanishing for $v_{\parallel} \rightarrow \pm\infty$.

7.3 FIELD PARTICLE OPERATOR

It is straightforward to show that the test particle operator does not conserve momentum and energy (cf. Helander and Sigmar, 2002), as is desirable for a physical collision model. The inclusion of the field particle operator ensures

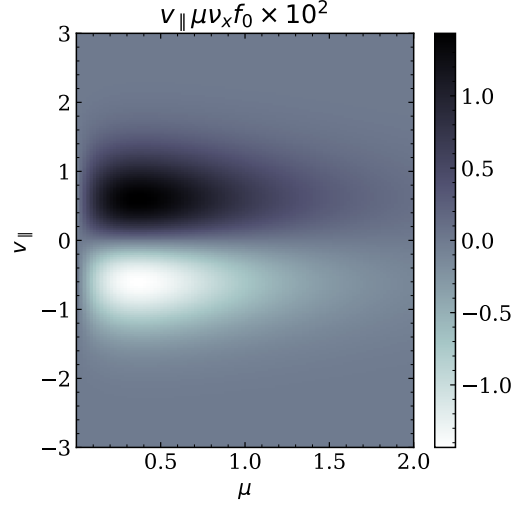


Figure 7.2: Collision frequency term occurring in the mixed-derivative terms of the test particle operator (7.21), for like-species collisions. The term vanishes for $\mu \rightarrow 0$ and $\mu \rightarrow \infty$, and for $v_{\parallel} \rightarrow \pm\infty$.

that these quantities are conserved for the combined collision operator. After linearisation of the collision operator, the field particle component can be written as

$$C_{\text{field}}^{ab}[F_{0a}, f_{b1}] = \frac{\partial}{\partial v_k} \left[L^{ab} \left(1 + \frac{m_a}{m_b} \right) \frac{\partial \phi_{b1}}{\partial v_k} F_{0a} + \frac{\partial}{\partial v_l} \left(-L^{ab} \frac{\partial^2 \psi_{b1}}{\partial v_k \partial v_l} F_{0a} \right) \right], \quad (7.23)$$

where the Rosenbluth potentials are now integral functionals of the perturbed distribution f_{b1} . Instead of dealing with the integro-differential operator of Eq. (7.23), gyrokinetic codes commonly replace the full field particle operator with an *ad hoc* operator designed to offset the momentum and energy produced by the test particle component to ensure overall momentum and energy conservation (Abel et al., 2008; Barnes et al., 2009; Sugama et al., 2009; Belli and Candy, 2011). In weakly collisional regimes this is acceptable, but inevitably becomes inaccurate for high collisionalities.

A rigorous approximation of the field operator can be obtained by performing a series expansion of the operator itself or the perturbed distribution function.

Hirshman and Sigmar (1976) developed such an expansion that has several desirable properties that will be discussed. In this section, we describe this model, convert it into a form compatible with the gyrokinetic equation and describe the implementation.

7.3.1 SPHERICAL HARMONIC EXPANSION

The spherical symmetry of collisions in a plasma motivates an expansion of the distribution function in spherical harmonics; indeed we will see that these are eigenfunctions of the collision operator (cf. Hirshman and Sigmar, 1976; Helander and Sigmar, 2002). Expanding the perturbed piece of the distribution function f_{b1} accordingly

$$f_{b1} = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} f_b^{(lm)}(v) Y_{lm}(\theta, \phi), \quad (7.24)$$

with expansion coefficients

$$f_b^{(lm)}(v) = \int \int f_{b1}(v, \theta, \phi) Y_{lm}^*(\theta, \phi) \sin \theta d\theta d\phi, \quad (7.25)$$

the field particle operator becomes

$$C_{\text{field}}^{ab}[F_{0a}, f_{b1}] = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} Y_{lm}(\theta, \phi) C_v^{ab} \left[f_b^{(lm)}(v) \right], \quad (7.26)$$

where C_v^{ab} is an isotropic operator that will be addressed shortly. The expansion in spherical harmonics has a useful implication for the velocity moments of the collision operator: the k -th velocity moment is given by

$$\begin{aligned} \int \mathbf{v}^k C_{ab}[F_{0a}, f_{b1}] d\mathbf{v} &= \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \int \hat{\mathbf{v}}^k Y_{lm}(\theta, \phi) \sin \theta d\theta d\phi \\ &\quad \times \int v^k C_v^{ab} \left[f_b^{(lm)}(v) \right] v^2 dv \\ &= \sum_{l=0}^k \sum_{m=-l}^{+l} \int \mathbf{v}^k Y_{lm}(\theta, \phi) C_v^{ab} \left[f_b^{(lm)}(v) \right] d^3v, \end{aligned} \quad (7.27)$$

where we used that $\hat{\mathbf{v}}^k$ can be expressed as a series of spherical harmonics up to degree k and the orthogonality of the spherical harmonics. Retaining the first k terms in the spherical harmonic expansion is thus sufficient to exactly represent the first $k + 1$ moments of the isotropic field particle operator. For notational clarity, we suppress the m -indices of the spherical harmonic expansion in what follows.

7.3.2 HIRSHMAN-SIGMAR EXPANSION OF THE ISOTROPIC OPERATOR

The isotropic operator $C_v^{ab}[f_b^{lm}]$ remains complicated. A common method in transport calculations is to expand the coefficients $f_b^{(l)}(v)$ around a Maxwellian in associated Laguerre polynomials $L_j^{(k)}(v^2)$ (Hirshman and Sigmar, 1976)

$$f_b^{(l)}(v) = \sum_{j=0}^{\infty} \frac{2}{v_{th,b}^{2l}} F_j^{(l)} v^l L_j^{(k)}(x_b^2) F_{0b}(x_b^2), \quad (7.28)$$

where $x_b := v/v_{th,b}$. The expansion coefficients, $F_j^{(l)}$, are then given by (Hirshman and Sigmar, 1976)

$$F_j^{(l)} = \frac{\pi^{3/2} j!}{(j + l + \frac{1}{2})!} \int_0^{\infty} v^l L_j^{(k)}(x_b^2) f_b^{(l)}(v) v^2 dv. \quad (7.29)$$

To satisfy the orthogonality relation of the Laguerre polynomials

$$\int_0^{\infty} L_m^{(k)}(x) L_n^{(k)}(x) x^k e^{-x} dx = \frac{(n+k)!}{n!} \delta(n-m), \quad (7.30)$$

the index of the Laguerre polynomials in Eq. (7.28) must be $k = l + \frac{1}{2}$.

Substituting the expansion given by Eq. (7.28) into the operator C_v^{ab} one obtains

$$C_v^{ab} [f_b^{(l)}(v)] = \frac{2}{v_{th,b}^{2l}} \sum_{j=0}^{\infty} F_j^{(l)} C_v^{ab} [x_b^l L_j^{(l+\frac{1}{2})}(x_b^2) F_{0b}(x_b^2)]. \quad (7.31)$$

An approximation to the field particle operator can be thus obtained by truncating the above series at a finite $j_{max} = N$. Usefully, the truncated series

vanishes on a Maxwellian distribution function, as can be verified by invoking the orthogonality relation of the Laguerre polynomials in Eq. (7.29), thus preserving the kernel of the exact field particle operator. However, the approximate operator does not correctly recover the velocity moments of the exact field particle operator since, for the k -th moment to be correctly given by the truncated expansion would require

$$\begin{aligned} \int_0^\infty v^k C_v^{ab} \left[f_b^{(l)}(v) \right] v^2 dv &= \frac{2}{v_{th,b}^l} \sum_{j=0}^N F_j^{(l)} [f_b^{(l)}] \\ &\times \int_0^\infty v^k C_v \left[x_b^l L_j^{(l+\frac{1}{2})}(x_b^2) F_{0b}(x_b^2) \right] v^2 dv, \end{aligned} \quad (7.32)$$

for arbitrary functions $f_b^{(l)}$. For $N = 0$ and $k = 1$ it follows immediately that this can only hold if the expansion coefficient $F_{j=0}^{(l)}[f_b^{(l)}]$ is a moment of the field particle operator. For $N > 0$ and $k > 1$ it follows inductively that all coefficients must be moments of the collision operator. Hirshman and Sigmar (1976) developed a modified expansion, that if truncated, guarantees the preservation of a subset of moments of the exact field particle operator. The method relies on a modified expansion of C_v^{ab} itself, as opposed to an expansion of the harmonic coefficients $f_b^{(l)}$. We assume a general series expansion of the operator C_v^{ab} , truncated at $j = N$, of the form

$$C_v^{ab,N} \left[f_b^{(l)}(v) \right] = \sum_{j=0}^N \psi_j^{ab,l} \Delta_j^{ab} \left[x_b^l L_j^{(l+\frac{1}{2})}(x_b^2) F_{0b}(x_b^2) \right],$$

where the scalars $\psi_j^{ab,l}$ are the expansion coefficients of the basis functions Δ_j^{ab} . Demanding that this series correctly give the l -th moment of the exact field particle operator

$$\begin{aligned} \int v^l C_v^{ab,N} \left[f_b^{(l)} \right] v^2 dv &= \\ \sum_{j=0}^N \psi_j^{ab,l} \int v^l \Delta_j^{ab} \left[x_b^l L_j^{(l+\frac{1}{2})}(x_b^2) F_{0b}(x_b^2) \right] v^2 dv, \end{aligned} \quad (7.33)$$

implies the condition,

$$\sum_{j=N+1}^{\infty} \psi_j^{(l)} \int v^l \Delta_j^{ab} \left[x_b^l L_j^{(l+\frac{1}{2})}(x_b^2) F_{0b}(x_b^2) \right] v^2 dv = 0. \quad (7.34)$$

This condition is always satisfied if the functions

$$\Delta_j^{ab,l} := \Delta_j^{ab} \left[x_b^l L_j^{(l+\frac{1}{2})}(x_b^2) F_{0b}(x_b^2) \right] \quad (7.35)$$

are orthogonal to the l -th velocity moment. A modified Gram-Schmidt orthogonalisation process is used to construct a set of Δ_j^{ab} with this property. Setting $\Delta_0^{ab}[f] = C_v^{ab}[f]$, the subsequent Δ_j are defined recursively as (Hirshman and Sigmar, 1976)

$$\Delta_{j+1}^{ab}[f] = \Delta_j^{ab}[f] - \psi_j^{ab,l}[f] \Delta_j^{ab,l}. \quad (7.36)$$

The requirement for orthogonality then determines the coefficients $\psi_j^{ab,l}$ to be given by

$$\psi_j^{ab,l}[f] = \frac{\int_0^\infty x_a^l \Delta_j^{ab}[f] v^2 dv}{\int_0^\infty x_a^l \Delta_j^{ab,l} v^2 dv}. \quad (7.37)$$

It is desirable that the operators Δ_j^{ab} are self-adjoint, so that the truncated approximate operator $C_v^{ab,N}$ retains the self-adjointness of the exact field particle operator. For any two functions h and g , the self-adjointness condition of the collision operator (cf. Helander and Sigmar, 2002) requires

$$\psi_j^{ab,l} [h F_{0b}] \int g \Delta_j^{ab,l} d^3v = \psi_j^{ab,l} [g F_{0b}] \int h \Delta_j^{ab,l} d^3v.$$

To enforce this condition the expansion coefficients can be modified as

$$\psi_j^{ab,l}[f_b] = \frac{\int_0^\infty x_a^l L_j^{(l+\frac{1}{2})}(x_a^2) \Delta_j^{ab}[f_b] v^2 dv}{\int_0^\infty x_a^l L_j^{(l+\frac{1}{2})}(x_a^2) \Delta_j^{ab,l} v^2 dv}, \quad (7.38)$$

that is, the functions Δ_{j+1}^{ab} are orthogonalised against the polynomial $v^l L_j^{(l+\frac{1}{2})}(x_a^2)$.

7.3.3 CONVERGENCE

We now prove that the constructed series expansion converges to the field particle operator. Rearranging the recursive definition (7.36) as

$$\Delta_j^{ab}[x_b^l L_j^{l+\frac{1}{2}} F_{0b}] = \left(\Delta_j^{ab}[x_b^l L_{j+1}^{l+\frac{1}{2}} F_{0b}] - \Delta_{j+1}^{ab}[x_b^l L_{j+1}^{l+\frac{1}{2}} F_{0b}] \right) / \psi_j^{ab}[x_b^l L_{j+1}^{l+\frac{1}{2}} F_{0b}], \quad (7.39)$$

and using the orthogonality relation

$$\int v^l L_{j-1}^{(l+\frac{1}{2})}(x_a^2) \Delta_j^{ab} v^2 dv = 0 \quad (7.40)$$

one obtains

$$\int v^l L_{j-1}^{(l+\frac{1}{2})}(x_a^2) \left(\Delta_j^{ab}[x_b^l L_{j+1}^{(l+\frac{1}{2})} F_{0b}] - \Delta_{j+1}^{ab}[x_b^l L_{j+1}^{(l+\frac{1}{2})} F_{0b}] \right) v^2 dv = 0. \quad (7.41)$$

Again using the orthogonality relation it follows that

$$\int v^l L_{j-1}^{(l+\frac{1}{2})}(x_a^2) \Delta_{j+1}^{ab}[x_b^l L_{j+1}^{(l+\frac{1}{2})} F_{0b}] v^2 dv = 0, \quad (7.42)$$

and by induction

$$\int v^l L_j^{(l+\frac{1}{2})}(x_a^2) \Delta_N^{ab}[x_b^l L_N^{(l+\frac{1}{2})} F_{0b}] v^2 dv = 0, \quad \text{for } j < N. \quad (7.43)$$

Writing out the recursive definition of Δ_j^{ab} (7.36) after $j+1-k$ steps one obtains

$$\Delta_{j+1}^{ab}[f] = \Delta_k^{ab}[f] - \sum_{i=k}^j \psi_i^{ab}[f] \Delta_i^{ab,l}. \quad (7.44)$$

It follows that for $k < j$

$$\begin{aligned} \Delta_j^{ab}[x_b^l L_k^{l+\frac{1}{2}} F_{0b}] &= \Delta_k^{ab}[x_b^l L_k^{l+\frac{1}{2}} F_{0b}] - \sum_{i=k}^{j-1} \frac{\int v^l L_k^{l+\frac{1}{2}} \Delta_i^{ab}[x_b^l L_i^{l+\frac{1}{2}} F_{0b}] v^2 dv}{\int v^l L_i^{l+\frac{1}{2}} \Delta_i^{ab}[x_b^l L_i^{l+\frac{1}{2}} F_{0b}] v^2 dv} \Delta_i^{ab,l}[x_b^l L_i^{l+\frac{1}{2}} F_{0b}] \\ &= - \sum_{i=k+1}^{j-1} \frac{\int v^l L_k^{l+\frac{1}{2}} \Delta_i^{ab}[x_b^l L_i^{l+\frac{1}{2}} F_{0b}] v^2 dv}{\int v^l L_i^{l+\frac{1}{2}} \Delta_i^{ab}[x_b^l L_i^{l+\frac{1}{2}} F_{0b}] v^2 dv} \Delta_i^{ab,l}[x_b^l L_i^{l+\frac{1}{2}} F_{0b}] \end{aligned} \quad (7.45)$$

Invoking the orthogonality (7.43) yields

$$\Delta_j^{ab}[x_b^l L_k^{l+\frac{1}{2}} F_{0b}] = 0 \quad \text{for } k < j. \quad (7.46)$$

Taking $k = 0$ in (7.44) and rearranging, the exact isotropic component of the field particle operator can be written as

$$\begin{aligned} C_v^{ab}[f] &:= \Delta_0^{ab}[f] = \sum_{j=0}^N \psi_j^{ab,l}[f] \Delta_j^{ab,l} + \Delta_{N+1}^{ab}[f] \\ &= C_v^{ab,N}[f] + \Delta_{N+1}^{ab}[f]. \end{aligned} \quad (7.47)$$

It follows immediately with (7.46) that the truncated operator $C_v^{ab,N}$ thus defined is exact for distribution functions of the form (Hirshman and Sigmar, 1976)

$$f_b^{(l)}(v) = \sum_{j=0}^N \frac{2}{v_{th,b}^{2l}} F_j^{(l)} v^l L_j^{(k)}(x_b^2) F_{0b}(x_b^2). \quad (7.48)$$

Since in the limit $N \rightarrow \infty$ any distribution function can be written in this way the approximate operator $C_v^{ab,N}(f)$ indeed converges to the exact field particle operator for $N \rightarrow \infty$ (Hirshman and Sigmar, 1976). The first element $\Delta_{j=0}^{ab,l}[x_b^l F_{0b}] = C_v^{ab}[x_b^l F_{0b}]$ in the series is calculated explicitly in the following section.

7.3.4 CALCULATION OF Δ_0

It remains to calculate the first element of the Hirshman-Sigmar expansion series, $\Delta_0^{l,ab}[x_b^l L_j^{(l+\frac{1}{2})}(x_b^2) F_{0b}] = C_v^{ab}[x_b^l L_j^{(l+\frac{1}{2})}(x_b^2) F_{0b}]$, where C_v^{ab} is the isotropic component of the field particle operator. The full field particle operator for collisions of f_b with F_{0a} is given by (cf. Helander and Sigmar, 2002)

$$\begin{aligned} C[f_{a_0}, f_{b_1}] &= L^{ab} F_{0a} \left[\frac{m_a}{m_b} f_{b_1}(v) + 2 \frac{v}{v_\alpha^2} \left(1 - \frac{m_a}{m_b} \right) \frac{\partial \phi_{b_1}}{\partial v} \right. \\ &\quad \left. + \frac{2}{v_\alpha^2} \phi_{b_1}(v) - \left(\frac{2v}{v_\alpha^2} \right)^2 \frac{\partial^2 \psi_{b_1}}{\partial v^2} \right]. \end{aligned} \quad (7.49)$$

We expand the Rosenbluth potentials in spherical harmonics, by using the generating function of the Legendre polynomials, P_l

$$\begin{aligned} \frac{1}{|\vec{v} - \vec{v}'|} &= \frac{1}{v \sqrt{1 + v'^2/v^2 - 2v'/v \cos \gamma}} \\ &= \frac{1}{v} \sum_{l=0}^{\infty} \left(\frac{v'}{v} \right)^l P_l(\cos \gamma), \end{aligned} \quad (7.50)$$

where $v' < v$ is required for convergence of the Legendre series, and γ denotes the angle between $\vec{v}$ and $\vec{v}'$. Using the addition theorem for the spherical harmonics it follows that

$$\frac{1}{|\vec{v} - \vec{v}'|} = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \frac{4\pi}{2l+1} (-1)^m \frac{v_{<}^l}{v_{>}^{l+1}} Y_l^{-m}(\theta, \phi) Y_l^m(\theta', \phi'), \quad (7.51)$$

with $v_{<} := \min(v, v')$ and $v_{>} := \max(v, v')$. The first Rosenbluth potential is then given by

$$\begin{aligned} \phi_b(\vec{v}) &= -\frac{1}{4\pi} \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \frac{4\pi}{2l+1} (-1)^m \left[Y_l^{-m}(\theta, \phi) \right. \\ &\quad \left. \int \int Y_l^m(\theta', \phi') \left(\frac{1}{v'^{l+1}} \int_0^v v'^{l+2} f_b(\vec{v}') dv' \right. \right. \\ &\quad \left. \left. + v^l \int_v^{\infty} \frac{1}{v'^{l-1}} f_b(\vec{v}') dv' \right) d\Omega' \right]. \end{aligned} \quad (7.52)$$

Using the orthogonality of the spherical harmonics it follows that for $f_b(\vec{v}) = f^{lm}(v) Y_l^m(\theta, \phi)$

$$\begin{aligned} \phi_b(\vec{v}) &= -\frac{1}{4\pi} \frac{4\pi}{2l+1} Y_l^m(\theta, \phi) \left(\frac{1}{v^{l+1}} \int_0^v v'^{l+2} f^{lm}(v') dv' \right. \\ &\quad \left. + v^l \int_v^{\infty} \frac{f^{lm}(v')}{v'^{l-1}} dv' \right). \end{aligned} \quad (7.53)$$

It follows that

$$\begin{aligned} \frac{\partial \phi_b(\vec{v})}{\partial v} &= -\frac{1}{4\pi} \frac{4\pi}{2l+1} Y_l^m(\theta, \phi) \left(-\frac{l+1}{v^{l+2}} \int_0^v v'^{l+2} f^{lm}(v') dv' \right. \\ &\quad \left. + l v^{l-1} \int_v^{\infty} \frac{f^{lm}(v')}{v'^{l-1}} dv' \right). \end{aligned} \quad (7.54)$$

To expand the second Rosenbluth potential, we multiply Eq. (7.50) by $(1 + v'^2/v^2 - 2v'/v \cos \gamma)$ and use the recurrence relation for the Legendre polynomials, $(2l+1)xP_l(x) = (l+1)P_{l+1}(x) + lP_{l-1}(x)$, to obtain, after some algebra and shifting of the summation indices

$$|\vec{v} - \vec{v}'| = \sum_{l=0}^{\infty} \frac{v_{<}^l}{v_{>}^{l+1}} \left[\frac{v_{<}^2}{2l+3} - \frac{v_{>}^2}{2l-1} \right] P_l(\cos \gamma). \quad (7.55)$$

It follows that

$$\psi_b(\vec{v}) = -\frac{1}{8\pi} \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \frac{4\pi}{2l+1} (-1)^m Y_l^{-m}(\theta, \phi) \quad (7.56)$$

$$\cdot \int \int Y_l^m(\theta', \phi') \left(\frac{1}{v'^{l+1}} \int_0^v v'^{l+2} \left[\frac{v'^2}{2l+3} - \frac{v^2}{2l-1} \right] f_b(\vec{v}') dv' \right. \\ \left. + v^l \int_v^{\infty} \frac{1}{v'^{l-1}} \left[\frac{v^2}{2l+3} - \frac{v'^2}{2l-1} \right] f_b(\vec{v}') dv' \right) d\Omega. \quad (7.57)$$

Then, for a distribution function of the form $f_b(\vec{v}) = f^{lm}(v)Y_l^m(\theta, \phi)$

$$\frac{\partial^2 \psi_b(\vec{v})}{\partial v^2} = -\frac{1}{8\pi} \frac{4\pi}{2l+1} Y_l^m(\theta, \phi) \left[\frac{(l+1)(l+2)}{2l+3} \times \right. \\ \left(\frac{1}{v^{l+3}} \int_0^v v'^{l+4} f^{lm}(v') dv' + v^l \int_v^{\infty} \frac{f^{lm}(v')}{v'^{l-1}} dv' \right) \\ - \frac{l(l-1)}{2l-1} \left(\frac{1}{v'^{l+1}} \int_0^v v'^{l+2} f^{lm}(v') dv' \right. \\ \left. \left. + v^{l-2} \int_v^{\infty} \frac{f^{lm}(v')}{v'^{l-3}} dv' \right) \right], \quad (7.58)$$

whence the field particle operator is given by

$$\begin{aligned}
C[F_{0a}, f_b^{lm}(v)Y_l^m(\theta, \phi)] &= L^{ab}F_{0a}Y_l^m(\theta, \phi)\frac{1}{2l+1}\left[(2l+1)\mu_{ab}f_b^{lm}(v) - 2\frac{v}{v_\alpha^2}(1 - \mu_{ab})\right. \\
&\quad \times \left(-\frac{l+1}{v^{l+2}}\int_0^v v'^{l+2}f_b^{lm}(v')dv' + lv^{l-1}\int_v^\infty \frac{f_b^{lm}(v')}{v'^{l-1}}dv'\right) \\
&\quad - \frac{2}{v_\alpha^2}\left(\frac{1}{v^{l+1}}\int_0^v v'^{l+2}f_b^{lm}(v')dv' + v^l\int_v^\infty \frac{f_b^{lm}(v')}{v'^{l-1}}dv'\right) \\
&\quad + \frac{1}{2}\left(\frac{2v}{v_\alpha^2}\right)^2\left\{\frac{(l+1)(l+2)}{2l+3}\left(\frac{1}{v^{l+3}}\int_0^v v'^{l+4}f_b^{lm}(v')dv'\right.\right. \\
&\quad \left.+ v^l\int_v^\infty \frac{f_b^{lm}(v')}{v'^{l-1}}dv'\right) - \frac{l(l-1)}{2l-1}\left(\frac{1}{v^{l+1}}\int_0^v v'^{l+2}f_b^{lm}(v')dv'\right. \\
&\quad \left.+ v^{l-2}\int_v^\infty \frac{f_b^{lm}(v')}{v'^{l-3}}dv'\right)\left.\right\}\left.\right] \\
&= Y_l^m(\theta, \phi)C_v^{(l)}[f_b^{lm}(v)].
\end{aligned} \tag{7.59}$$

The spherical harmonics are therefore eigenfunctions of the field particle collision operator. The calculation of the basis functions $\Delta_j^{l+\frac{1}{2},ab}\left[x_b^l L_j^{(l+1/2)}(x_b^2)\exp(-x_b^2)\right]$ for the Hirshman-Sigmar expansion of the field particle operator requires the calculation of

$$\Delta_0^{l+\frac{1}{2},ab}\left[x_b^l L_j^{(l+1/2)}(x_b^2)\exp(-x_b^2)\right] = C_v^{ab}\left[F_{0a}, x_b^l L_j^{(l+1/2)}(x_b^2)\exp(-x_b^2)\right]. \tag{7.60}$$

The resulting integral expressions over Laguerre polynomials can be simplified by using the definition of the generalised Laguerre polynomials

$$L_j^{(l+\frac{1}{2})}(x) = \sum_{k=0}^j \underbrace{\frac{(-1)^k(l+j+1/2)!}{(j-k)!(l+k+1/2)!k!}}_{=:c_k^{jl}} x^k \tag{7.61}$$

After some algebra and introducing the lower and upper incomplete Gamma functions, $\gamma(s, x)$ and $\Gamma(s, x)$, respectively (cf. Gradshteyn and Ryzhik, 2007),

one obtains

$$\begin{aligned}
\Delta_0^{l+\frac{1}{2},ab} \left[x_b^l L_j^{l+1/2}(x_b^2) \exp(-x_b^2) \right] = \\
L^{ab} \mu_{ab} \exp(-x_a^2) \frac{1}{2l+1} \sum_{i=0}^j c_i^{jl} \left[(2l+1) x_b^{l+2i} \exp(-x_b^2) \right. \\
- x_b (1 - \mu_{ab}) \left(-\frac{l+1}{x_b^{l+2}} \gamma(3/2 + l + i, x_b^2) + l x_b^{l-1} \Gamma(1 + i, x_b^2) \right) \\
- \left(\frac{1}{x_b^{l+1}} \gamma(3/2 + l + i, x_b^2) + x_b^l \Gamma(1 + i, x_b^2) \right) \\
+ \mu_{ab} x_b^2 \frac{(l+1)(l+2)}{2l+3} \left(\frac{1}{x_b^{l+3}} \gamma(5/2 + l + i, x_b^2) + x_b^l \Gamma(1 + i, x_b^2) \right) \\
\left. - \mu_{ab} x_b^2 \frac{l(l-1)}{2l-1} \left(\frac{1}{x_b^{l+1}} \gamma(3/2 + l + i, x_b^2) + x_b^{l-2} \Gamma(2 + i, x_b^2) \right) \right]. \quad (7.62)
\end{aligned}$$

For the purpose of the implementation of the collision operator, discussed at length in the following chapter, the incomplete gamma functions can be calculated recursively from the error function that is available in **FORTRAN**, using the standard recursion formulae for integer parameters s

$$\gamma(s+1, x) = s\gamma(s, x) - x^s \exp(-x) \quad (7.63)$$

$$\Gamma(s+1, x) = s\Gamma(s, x) + x^s \exp(-x). \quad (7.64)$$

7.3.5 COMBINED EXPANSION OF THE FIELD-PARTICLE OPERATOR

Combining the results of this section, the Hirshman-Sigmar field particle operator is given by

$$C_{\text{field}}^{ab}[F_{0a}, f_{b1}] = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} Y_{lm}(\theta, \phi) C_v^{ab} \left[f_b^{(lm)}(v) \right], \quad (7.65)$$

where

$$f_b^{(lm)}(v) = \int \int f_{b1}(v, \theta, \phi) Y_{lm}^*(\theta, \phi) \sin \theta d\theta d\phi, \quad (7.66)$$

and

$$C_v^{ab} [f_b^{(lm)}] := \sum_{j=0}^{\infty} \psi_j^{ab,l} [f_b^{(lm)}] \Delta_j^{ab,l}, \quad (7.67)$$

with expansion coefficients $\psi_j^{ab,l}$ given by

$$\psi_j^{ab,l} [f_b^{(lm)}] = \frac{\int_0^{\infty} x_a^l L_j^{(l+\frac{1}{2})}(x_a^2) \Delta_j^{ab} [f_b^{(lm)}] v^2 dv}{\int_0^{\infty} x_a^l L_j^{(l+\frac{1}{2})}(x_a^2) \Delta_j^{ab,l} v^2 dv}. \quad (7.68)$$

The Hirshman-Sigmar operator has several useful properties: the accuracy of the approximation can be improved by successively increasing the number of terms in the series expansion, and by design, the operator recovers the first $N + 1$ velocity moments, preserves the null-space and retains the self-adjointness of the exact field particle operator.

7.4 GYROKINETIC FORM OF THE COLLISION OPERATOR

To be compatible with the gyrokinetic equation, the collision operator is gyroaveraged. To facilitate this, the distribution function can be written spectrally in components of the guiding-center $\mathbf{R}$ that are perpendicular to the magnetic field

$$h = \sum_{\mathbf{k}_{\perp}} e^{i\mathbf{k}_{\perp} \cdot \mathbf{R}} h_{\mathbf{k}_{\perp}}(z, v_{\parallel}, \mu), \quad (7.69)$$

where z denotes the spatial coordinate along the field line, $\mathbf{R} = \mathbf{r} - \boldsymbol{\rho}$, and $\mathbf{r}$, $\boldsymbol{\rho} = \hat{\mathbf{b}} \times \mathbf{v}/\Omega$ and Ω denote the particle position, Larmor vector and cyclotron frequency, respectively. We have suppressed species indices for brevity; these will be reintroduced later. The gyrokinetic collision operator then becomes (Abel et al., 2008)

$$\begin{aligned} C_{\text{GK}}[h] &= \left\langle C \left[\sum_{\mathbf{k}_{\perp}} e^{i\mathbf{k}_{\perp} \cdot \mathbf{R}} h_{\mathbf{k}_{\perp}} \right] \right\rangle = \sum_{\mathbf{k}_{\perp}} \langle e^{i\mathbf{k}_{\perp} \cdot \mathbf{r}} C[e^{-i\mathbf{k}_{\perp} \cdot \boldsymbol{\rho}} h_{\mathbf{k}_{\perp}}] \rangle_{\mathbf{R}} \\ &= \sum_{\mathbf{k}_{\perp}} e^{i\mathbf{k}_{\perp} \cdot \mathbf{R}} \langle e^{i\mathbf{k}_{\perp} \cdot \boldsymbol{\rho}} C[e^{-i\mathbf{k}_{\perp} \cdot \boldsymbol{\rho}} h_{\mathbf{k}_{\perp}}] \rangle_{\mathbf{R}}, \end{aligned} \quad (7.70)$$

where $\langle h \rangle = 1/(2\pi) \int_0^{2\pi} h \, d\phi$ denotes the gyroaverage, performed at fixed guiding-center $\mathbf{R}$. The Fourier components of the gyrokinetic collision operator are then given by

$$C_{\text{GK}}[h_{\mathbf{k}\perp}] = \langle e^{i\mathbf{k}\perp \cdot \boldsymbol{\rho}} C[e^{-i\mathbf{k}\perp \cdot \boldsymbol{\rho}} h_{\mathbf{k}\perp}] \rangle_{\mathbf{R}}. \quad (7.71)$$

7.4.1 GYROAVERAGED TEST-PARTICLE OPERATOR

We proceed to compute the Fourier components of the gyroaveraged test-particle operator expressed in $(v_{\parallel}, \mu)$ -coordinates. Since the gyro-average is taken at fixed guiding center $\mathbf{R}$, the velocity derivatives in the collision operator are first transformed to derivatives at fixed $\mathbf{R}$

$$\begin{aligned} \left. \frac{\partial}{\partial \phi} \right|_{\mathbf{r}} &= \left. \frac{\partial}{\partial \phi} \right|_{\mathbf{R}} + \left. \frac{\partial \mathbf{R}}{\partial \phi} \frac{\partial}{\partial \mathbf{R}} \right|_{\mathbf{v}} = \left. \frac{\partial}{\partial \phi} \right|_{\mathbf{R}} - \frac{1}{\Omega} \frac{\partial}{\partial \phi} (\hat{\mathbf{b}} \times \mathbf{v}_{\perp}) \left. \frac{\partial}{\partial \mathbf{R}} \right|_{\mathbf{v}} \\ &= \left. \frac{\partial}{\partial \phi} \right|_{\mathbf{R}} + \frac{\mathbf{v}_{\perp}}{\Omega} \cdot \left. \frac{\partial}{\partial \mathbf{R}} \right|_{\mathbf{v}} \end{aligned} \quad (7.72)$$

$$\begin{aligned} \left. \frac{\partial}{\partial \mu} \right|_{\mathbf{r}} &= \left. \frac{\partial}{\partial \mu} \right|_{\mathbf{R}} + \left. \frac{\partial \mathbf{R}}{\partial \mu} \frac{\partial}{\partial \mathbf{R}} \right|_{\mathbf{v}} = \left. \frac{\partial}{\partial \mu} \right|_{\mathbf{R}} - \frac{\hat{\mathbf{b}}}{\Omega} \times \frac{\partial \mathbf{v}_{\perp}}{\partial \mu} \left. \frac{\partial}{\partial \mathbf{R}} \right|_{\mathbf{v}} \\ &= \left. \frac{\partial}{\partial \mu} \right|_{\mathbf{R}} - \frac{1}{2\mu} \boldsymbol{\rho} \cdot \left. \frac{\partial}{\partial \mathbf{R}} \right|_{\mathbf{v}} \end{aligned} \quad (7.73)$$

$$\left. \frac{\partial}{\partial v_{\parallel}} \right|_{\mathbf{r}} = \left. \frac{\partial}{\partial v_{\parallel}} \right|_{\mathbf{R}} + \left. \frac{\partial \mathbf{R}}{\partial v_{\parallel}} \frac{\partial}{\partial \mathbf{R}} \right|_{\mathbf{v}} = \left. \frac{\partial}{\partial v_{\parallel}} \right|_{\mathbf{R}} \quad (7.74)$$

where we used that $\mu = mv_{\perp}^2/2B_0$, so that $\partial_{\mu} \mathbf{v}_{\perp} = \mathbf{v}_{\perp}/v_{\perp}^2 \cdot B_0/m = \mathbf{v}_{\perp}/\mu/2$. We now perform the gyro-averaging operation (7.71). The $v_{\parallel}$ -component of the collision operator is unaffected. Aligning $\mathbf{k}$ with the $\phi = 0$ axis

$$\begin{aligned} \frac{\partial}{\partial \mu} (e^{-i\mathbf{k} \cdot \boldsymbol{\rho}} h_{\mathbf{k}}) &= \frac{\partial}{\partial \mu} e^{-i\mathbf{k} \cdot (\hat{\mathbf{b}} \times \mathbf{v}_{\perp})/\Omega} h_{\mathbf{k}} = \frac{\partial}{\partial \mu} e^{ikv_{\perp} \sin \phi/\Omega} h_{\mathbf{k}} = \frac{\partial}{\partial \mu} e^{ik\sqrt{2B_0\mu/m} \sin \phi/\Omega} h_{\mathbf{k}} \\ &= ik \frac{B_0 \sin \phi}{mv_{\perp} \Omega} e^{ikv_{\perp} \sin \phi/\Omega} h_{\mathbf{k}} + e^{ikv_{\perp} \sin \phi/\Omega} \frac{\partial h_{\mathbf{k}}}{\partial \mu}. \end{aligned} \quad (7.75)$$

For the μ -component of the collision operator

$$\begin{aligned}
& \left\langle e^{i\mathbf{k}\cdot\boldsymbol{\rho}} \frac{\partial}{\partial\mu} \left([2\nu_{\parallel}\mu^2 + \nu_D\mu m v_{\parallel}^2/B_0] \left[ik \frac{B_0 \sin\phi}{m v_{\perp} \Omega} e^{-i\mathbf{k}\cdot\boldsymbol{\rho}} h_{\mathbf{k}} + e^{-i\mathbf{k}\cdot\boldsymbol{\rho}} \frac{\partial h_{\mathbf{k}}}{\partial\mu} \right] \right. \right. \\
& \quad \left. \left. + \nu_s \mu h_{\mathbf{k}} e^{-i\mathbf{k}\cdot\boldsymbol{\rho}} \right) \right\rangle \\
& = \frac{\partial}{\partial\mu} \left(2\nu_{\parallel}\mu^2 \frac{\partial h_{\mathbf{k}}}{\partial\mu} + \nu_s \mu h_{\mathbf{k}} + \nu_D\mu m v_{\parallel}^2/B_0 \frac{\partial h_{\mathbf{k}}}{\partial\mu} \right) - \frac{k^2}{4\Omega^2} \left[\nu_{\parallel} v_{\perp}^2 + \nu_D v_{\parallel}^2 \right] h_{\mathbf{k}}
\end{aligned} \tag{7.76}$$

where we used that $\langle \sin\phi \rangle = \langle \cos\phi \rangle = \langle \cos\phi \sin\phi \rangle = 0$. The mixed-differential components of the operator are unchanged because the gyro-average over $\boldsymbol{\rho}$ vanishes. For the ϕ -differential component of the operator

$$\begin{aligned}
& \left\langle e^{i\boldsymbol{\rho}\cdot\mathbf{k}} \frac{\nu_D}{2} \left(1 + \frac{m v_{\parallel}^2}{2B_0\mu} \right) \frac{\partial^2 e^{-i\boldsymbol{\rho}\cdot\mathbf{k}} h_{\mathbf{k}}}{\partial\phi^2} \right\rangle = \left\langle -\frac{\nu_D}{2} \left(1 + \frac{m v_{\parallel}^2}{2B_0\mu} \right) \frac{k_{\perp}^2 v_{\perp}^2 \cos^2\phi}{\Omega^2} \right\rangle \\
& = -\nu_D \frac{k_{\perp}^2 v_{\perp}^2}{4\Omega^2} h_{\mathbf{k}}.
\end{aligned} \tag{7.77}$$

Collecting the μ -, $v_{\parallel}$ - and ϕ -terms, the gyrokinetic test-particle collision operator in Fourier space is given by

$$\begin{aligned}
C_{\text{GK,test}}[h_{\mathbf{k}_{\perp}}] & = \frac{\partial}{\partial v_{\parallel}} \left[\gamma_{v_{\parallel}}^{ab} F_0 \frac{\partial}{\partial v_{\parallel}} \frac{h_{\mathbf{k}_{\perp}}}{F_0} + v_{\parallel} \mu \nu_x^{ab} F_0 \frac{\partial}{\partial\mu} \frac{h_{\mathbf{k}_{\perp}}}{F_0} \right] \\
& + \frac{\partial}{\partial\mu} \left[\gamma_{\mu}^{ab} F_0 \frac{\partial}{\partial\mu} \frac{h_{\mathbf{k}_{\perp}}}{F_0} + v_{\parallel} \mu \nu_x^{ab} F_0 \frac{\partial}{\partial v_{\parallel}} \frac{h_{\mathbf{k}_{\perp}}}{F_0} \right] \\
& - \frac{1}{2} \left(\nu_{\parallel} B_0 \mu + \nu_D [v_{\parallel}^2 + B_0 \mu] \right) k_{\perp}^2 \rho^2 h_{\mathbf{k}_{\perp}},
\end{aligned} \tag{7.78}$$

where we have again obtained a more compact form of the collision operator by acting on h/F_0 and where all velocity-space derivatives are now performed at fixed guiding-center. The gyroaverage of the collision operator has thus eliminated the dependence on the gyroangle and introduced a spatial diffusive term that is proportional to the square of the thermal Larmor radius, $\rho = v_{th}/\Omega$, and perpendicular wave number.

7.4.2 GYROAVERAGED FIELD-PARTICLE OPERATOR

Turning to the field particle operator we perform the expansion in spherical harmonics

$$e^{-i\mathbf{k}_\perp \cdot \boldsymbol{\rho}} h_{\mathbf{k}_\perp} = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} Y_{lm}(\theta, \phi) h_{\mathbf{k}_\perp}^{lm}(v), \quad (7.79)$$

with coefficients,

$$\begin{aligned} h_{\mathbf{k}_\perp}^{lm}(v) &= \int \int Y_{lm}^*(\theta, \phi) e^{-i\mathbf{k}_\perp \cdot \boldsymbol{\rho}} h_{\mathbf{k}_\perp}(z, v_\parallel, \mu) \sin \theta d\theta d\phi \\ &= c_{l,-m} \int \int (-1)^m e^{-im\phi + ikv_\perp \sin \phi / \Omega} d\phi P_{l,-m}(\cos \theta) h_{\mathbf{k}_\perp}(z, v_\parallel, \mu) \sin \theta d\theta \\ &= 2\pi c_{l,-m} (-1)^m \int \int J_m\left(\frac{k_\perp v_\perp}{\Omega}\right) P_{l,-m}(\cos \theta) h_{\mathbf{k}_\perp}(z, v_\parallel, \mu) \sin \theta d\theta, \end{aligned} \quad (7.80)$$

where P_{lm} are the associated Legendre polynomials and we have used that $Y_{lm}(\theta, \phi) = c_{lm} P_{lm}(\cos \theta) e^{im\phi}$ with $c_{lm} = \sqrt{\frac{(2l+1)(l-m)!}{(4\pi)(l+m)!}}$; $\mathbf{k}_\perp \cdot \boldsymbol{\rho} = -kv_\perp \sin \phi / \Omega$ and the Jacobi-Anger identity

$$J_n(x) = \frac{1}{2\pi} \int_0^{2\pi} e^{i(x \sin(\phi) - n\phi)} d\phi. \quad (7.81)$$

Then

$$\begin{aligned} C_{\text{GK,field}}[h_{\mathbf{k}_\perp}] &= \\ &= \sum_{\mathbf{k}_\perp} e^{i\mathbf{k}_\perp \cdot \mathbf{R}} \left\langle e^{i\mathbf{k}_\perp \cdot \boldsymbol{\rho}} C_{\text{field}} \left[\sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} Y_{lm}(\theta, \phi) h_{\mathbf{k}_\perp}^{lm}(v) \right] \right\rangle_{\mathbf{R}} \\ &= \sum_{\mathbf{k}_\perp} e^{i\mathbf{k}_\perp \cdot \mathbf{R}} \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} \langle e^{i\mathbf{k}_\perp \cdot \boldsymbol{\rho}} Y_{lm}(\theta, \phi) \rangle_{\mathbf{R}} C_v^{ab} [h_{\mathbf{k}_\perp}^{lm}(v)], \end{aligned} \quad (7.82)$$

where in the last line we used that the spherical harmonics are eigenfunctions of the collision operator and C_v^{ab} is the isotropic component of the Hirshman-Sigmar field particle operator. With

$$\begin{aligned} \langle e^{i\mathbf{k}_\perp \cdot \boldsymbol{\rho}} Y_{lm}(\theta, \phi) \rangle_{\mathbf{R}} &= \frac{1}{2\pi} \int_0^{2\pi} e^{i\mathbf{k}_\perp \cdot \boldsymbol{\rho}} Y_{lm} d\phi \\ &= c_{lm} P_{lm}(\cos \theta) \frac{1}{2\pi} \int_0^{2\pi} e^{-ikv_\perp \sin \phi / \Omega + im\phi} d\phi \end{aligned} \quad (7.83)$$

it follows that the k -th Fourier component of the field particle operator is given by

$$\begin{aligned}
C_{\text{GK,field}}[h_{\mathbf{k}_\perp}] &= \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} c_{lm} P_{lm}(\cos \theta) J_m \left(\frac{k_\perp v_\perp}{\Omega} \right) C_v [h_{\mathbf{k}_\perp}^{lm}(v)] \\
&= \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} \sum_{j=0}^{\infty} c_{lm} P_{lm}(\cos \theta) J_m \left(\frac{k_\perp v_\perp}{\Omega} \right) \psi_j^l [h_{\mathbf{k}_\perp}^{lm}(v)] \\
&\quad \times \Delta_j \left(x^l L_j^{(l+1/2)}(x^2) F_0 \right). \tag{7.84}
\end{aligned}$$

The coefficients ψ_j^l are given by

$$\begin{aligned}
\psi_j^l [h_{\mathbf{k}_\perp}^{lm}(v)] &= 2\pi c_{l,-m} (-1)^m \frac{1}{N_j^l} \int \int P_{l,-m}(\cos \theta) J_m \left(\frac{k_\perp v_\perp}{\Omega} \right) \\
&\quad \times h_{\mathbf{k}_\perp} \Delta_j^{(l)} \left[x^l L_j^{(l+1/2)}(x^2) F_0(x) \right] v^2 dv \sin \theta d\theta \tag{7.85}
\end{aligned}$$

where $x = v/v_{th}$, species indices are suppressed and N_j^l is the normalisation $N_j^l := \int \int x^l L_j^{(l+1/2)}(x^2) \Delta_j^l [x^l L_j^{(l+1/2)} F_0(x)] v^2 dv \sin \theta d\theta$. In writing Eq. (7.85) we have used the self-adjointness of the operators $\Delta_j^{(l)}$ to obtain $\int x^l L_j^{(l+1/2)}(x^2) \Delta_j^{(l)} [h_{\mathbf{k}}^{lm}] v^2 dv = \int h_{\mathbf{k}}^{lm} / F_0(x) \Delta_j^{(l)} [x^l L_j^{(l+1/2)}(x^2) F_0(x)] v^2 dv$. For the purpose of the numerical implementation one can combine positive and negative m -indices in (7.84) by using $P_{l,-m} = (-1)^m (l-m)! / (l+m)! P_{lm}$ and $J_{-m} = (-1)^m J_m$, whence

$$\begin{aligned}
C_{\text{GK,field}}[h_{\mathbf{k}_\perp}] &= \sum_{l=1}^{\infty} c_{l,0} P_{l,0}(\cos \theta) J_0 \left(\frac{k_\perp v_\perp}{\Omega} \right) C_v [h_{\mathbf{k}_\perp}^{l,0}(v)] \\
&\quad + 2 \sum_{m=1}^{m=+l} c_{lm} P_{lm}(\cos \theta) J_m \left(\frac{k_\perp v_\perp}{\Omega} \right) C_v [h_{\mathbf{k}_\perp}^{lm}(v)]. \tag{7.86}
\end{aligned}$$

With this in hand, we turn to the numerical implementation of the collision model.

CHAPTER 8

NUMERICAL IMPLEMENTATION IN stella

In this chapter, we discuss the implementation of the collision model in the gyrokinetic code `stella`.

8.1 VELOCITY SPACE DISCRETISATION

The gyrokinetic code `stella` (Barnes et al., 2018) advances the gyrokinetic equation in terms of the distribution function $g = \langle \delta f \rangle = h - \frac{q}{T} \langle \phi \rangle F_0$, where, to be clear, ϕ denotes the electrostatic potential, not the gyroangle, as in the previous chapter. The code discretizes velocity-space quantities on a uniformly spaced $v_{\parallel}$ -grid and optionally uses either a uniform or Gauss-Laguerre grid for the magnetic moment $\mu = mv_{\perp}^2/2B$. Discretisation and integration schemes in the code should ideally be chosen such that the conservation laws and the self-adjointness of the collision operator are retained in the numerical implementation. The single-variable double derivative terms in Eq. (7.78) are of the form $d/dx[G(x, y)dh/dx]$, where $G(x, y)$ is a function specific to the $v_{\parallel}$ - or μ -term, and $x, y \in \{v_{\parallel}, \mu\}$. The self-adjointness of the single-variable double-derivative terms then follows immediately upon double integration by parts and use of the boundary conditions. For the mixed-derivative terms in

the test-particle operator, that are of the form $d/dx[G(x, y)dh/dy]$ we have, for $(x, y) = (v_{\parallel}, \mu)$ or $(x, y) = (\mu, v_{\parallel})$ that

$$\begin{aligned} \int \int f \frac{\partial}{\partial x} \left[G(x, y) \frac{\partial h}{\partial y} \right] dx dy &= - \int \int \frac{\partial f}{\partial x} \left[G(x, y) \frac{\partial h}{\partial y} \right] dx dy \\ &= \int \int h \frac{\partial}{\partial y} \left[G(x, y) \frac{\partial f}{\partial x} \right] dx dy, \end{aligned} \quad (8.1)$$

where we have integrated by parts in x and y , and used that the distribution function h vanishes at infinity. Thus, taken together, the two mixed derivative terms in the test particle operator are self-adjoint, and the combined test-particle operator is self-adjoint.

8.1.1 UNIFORM VELOCITY GRIDS

The $v_{\parallel}$ -grid in **stella** is anti-symmetric around $v_{\parallel} = 0$. The point $v_{\parallel} = 0$ is not included in the grid. The uniform μ -grid is chosen such that the smallest μ -value, μ_{min} is given by $\mu_{min} = \Delta_{\mu}/2$, where Δ_{μ} denotes the grid spacing. The maximum parallel velocity and magnetic moment are parameters that can be set by the user. Derivatives in the test particle operator given by Eq. (7.78) are discretized using a three-point stencil for both velocity-space grids. Then, at index i , and suppressing the second index j , the derivative is approximated by

$$\frac{\partial}{\partial x} \left[G(x) \frac{\partial h}{\partial x} \right]_i \approx \frac{1}{\Delta} \left[-G(x_{i-\frac{1}{2}}) \left(\frac{\partial h}{\partial x} \right)_{i-\frac{1}{2}} + G(x_{i+\frac{1}{2}}) \left(\frac{\partial h}{\partial x} \right)_{i+\frac{1}{2}} \right], \quad (8.2)$$

with $(\partial h/\partial x)_{i-\frac{1}{2}} = (h_i - h_{i-1})/\Delta$ and analogously for $(\partial h/\partial x)_{i+\frac{1}{2}}$. Here $x_{i+1/2} = (x_i + x_{i+1})/2$ and $x_{i-1/2} = (x_i - x_{i+1})/2$, and $G_{i\pm 1/2} = G(x_{i\pm 1/2})$. The discretisation scheme (8.2) is second order accurate (cf. Barnes et al., 2009).

At boundaries $i = \{1, N\}$, it is assumed that $G_{N+1/2} = 0$ and $G_{1-1/2} = 0$. This is justified by the asymptotics of the function $G(x, y)$ (cf. Section 7.2,

Figures 7.1 and 7.2). It follows immediately that the sum

$$\sum_{i=1}^N \left[-G\left(x_{i-\frac{1}{2}}\right) \left(\frac{\partial h}{\partial x}\right)_{i-\frac{1}{2}} + G\left(x_{i+\frac{1}{2}}\right) \left(\frac{\partial h}{\partial x}\right)_{i+\frac{1}{2}} \right] = 0, \quad (8.3)$$

since the terms in the sum telescope and terms beyond the boundary indices vanish. Eq. (8.3) implies that the discrete density integral of the terms discretised with the scheme (8.2) vanishes exactly – that is, independently of the velocity-space resolution – as is required for exact density conservation of the collision operator. If the weights of the integration scheme employed are uniform, the discretisation of the single-variable double derivative terms given by (8.2) satisfies the numerical equivalents of integration by parts and the fundamental theorem of calculus. This can be readily verified by multiplying (8.2) by a test function, summing the index from $i = 1$ to $i = N$ and shifting summation indices where opportune. It follows that (8.2) is self-adjoint. With the discretisation scheme the coefficient of h_i is

$$\frac{1}{\Delta_i^2} (G_{i+1/2} - G_{i-1/2}), \quad (8.4)$$

and the coefficients of h_{i+1} and h_{i-1} are

$$\frac{1}{\Delta_i^2} G_{i+1/2} \quad (8.5)$$

and

$$-\frac{1}{\Delta_i^2} G_{i-1/2}, \quad (8.6)$$

respectively, where the second index, j , is suppressed everywhere. The analogous scheme is employed for the term $\partial/\partial y (G(y) \partial h / \partial y)$ with index j .

The mixed derivative terms in Eq. (7.78) may be discretised using a standard centered difference

$$\begin{aligned} \frac{\partial}{\partial x} \left[G(x, y) \frac{\partial h}{\partial y} \right]_{i,j} &\approx \left[-G(x_{i-1}, y_j) \left(\frac{\partial h}{\partial y} \right)_{i-1,j} \right. \\ &\quad \left. + G(x_{i+1}, y_j) \left(\frac{\partial h}{\partial y} \right)_{i+1,j} \right] \frac{1}{2\Delta_i}, \end{aligned} \quad (8.7)$$

with

$$\left(\frac{\partial h}{\partial y}\right)_{i-1,j} = \frac{h_{i-1,j+1} - h_{i-1,j-1}}{2\Delta_j}, \quad (8.8)$$

and analogously for $(\partial h/\partial y)_{i+1,j}$. However, this scheme fails to guarantee density conservation and self-adjointness of the test particle operator, as can be verified by multiplying by a test function and integrating by parts. A scheme that has this property is given by

$$\frac{\partial}{\partial v_{\parallel}} \left[G \frac{\partial h}{\partial \mu} \right]_{i,j} \approx \left[G_{i+1/2,j} \left(\frac{\partial h}{\partial \mu} \right)_{i+1/2,j} - G_{i-1/2,j} \left(\frac{\partial h}{\partial \mu} \right)_{i-1/2,j} \right] / \Delta v_{\parallel}, \quad (8.9)$$

where $h_{i\pm 1/2,j} = (h_{i,j} + h_{i\pm 1,j})/2$, the inner derivative is approximated by

$$G_{i\pm 1/2,j} \left(\frac{\partial h}{\partial \mu} \right)_{i\pm 1/2,j} \approx \frac{1}{2} \left[G_{i\pm 1/2,j+1/2} \frac{h_{i\pm 1/2,j+1} - h_{i\pm 1/2,j}}{\Delta_{\mu}} + G_{i\pm 1/2,j-1/2} \frac{h_{i\pm 1/2,j} - h_{i\pm 1/2,j-1}}{\Delta_{\mu}} \right], \quad (8.10)$$

and G is assumed to vanish at half-indices beyond the boundaries. Upon summation, density conservation follows immediately from the telescoping property of the series and boundary conditions. With this scheme the coefficient of $h_{i,j}$ is

$$\frac{1}{4\Delta_{\mu}\Delta v_{\parallel}} \left[(-G_{i+1/2,j+1/2} + G_{i+1/2,j-1/2}) - (-G_{i-1/2,j+1/2} + G_{i-1/2,j-1/2}) \right], \quad (8.11)$$

and the coefficients of $h_{i,j\pm 1}$ are

$$\frac{1}{4\Delta_{\mu}\Delta v_{\parallel}} \left[\mp G_{i+1/2,j\pm 1/2} \pm G_{i-1/2,j\pm 1/2} \right]. \quad (8.12)$$

For $h_{i\pm 1,j+1}$ one obtains

$$\pm \frac{1}{4\Delta_{\mu}\Delta v_{\parallel}} (-G_{i\pm 1/2,j+1/2}), \quad (8.13)$$

for $h_{i\pm 1,j-1}$

$$\pm \frac{1}{4\Delta_\mu \Delta v_\parallel} (G_{i\pm 1/2,j-1/2}), \quad (8.14)$$

and for $h_{i\pm 1,j}$ the coefficients are

$$\pm \frac{1}{4\Delta_\mu \Delta v_\parallel} (-G_{i\pm 1/2,j+1/2} + G_{i\pm 1/2,j-1/2}). \quad (8.15)$$

The same scheme is used to discretise the term $\partial/\partial\mu(G\partial h/\partial v_\parallel)$.

We now construct a discretisation matrix of the test particle operator that we will require for an implementation of the collision operator discussed in Section 8.2. The single-variable $v_\parallel$ - and μ -differential terms may be represented using tridiagonal matrices of dimension $N_{v_\parallel} \times N_{v_\parallel}$ and $N_\mu \times N_\mu$ that we denote as $C_{v_\parallel}''$ and C_μ'' . For the mixed-differential components of the test particle operator we define the tridiagonal operators $C_\mu^*[\cdot] := \partial/\partial\mu[v_\parallel\mu\nu_x F_0\cdot]$ and $C_{v_\parallel}[\cdot] := \partial/\partial v_\parallel[\cdot]$, with $C_{v_\parallel}^*$ and C_μ defined analogously. We can then write the combined mixed-differential operator, $C_{v_\parallel\mu}$, acting on $h^T \in \mathbb{R}^{N_\mu \times N_{v_\parallel}}$ – the choice to operate on h^T will be motivated shortly – as

$$C_{v_\parallel\mu}[h^T] = C_\mu h^T C_{v_\parallel}^{*T} + C_\mu^* h^T C_{v_\parallel}^T. \quad (8.16)$$

With $\text{vec}(ABC) = (C^T \otimes A)\text{vec}(B)$, where $\otimes$ denotes the Kronecker product, one obtains

$$\text{vec}(C_{v_\parallel\mu}[h^T]) = [C_{v_\parallel}^* \otimes C_\mu + C_{v_\parallel} \otimes C_\mu^*]\text{vec}(h^T), \quad (8.17)$$

where $\text{vec}(h^T)$ is a $N_\mu N_{v_\parallel} \times 1$ -column vector obtained by stacking the columns of h^T . Combining the mixed-differential terms with the single variable terms, the test particle operator is represented by the matrix

$$C_{\text{test}} = C_{v_\parallel}^* \otimes C_\mu + C_{v_\parallel} \otimes C_\mu^* + I_{v_\parallel} \otimes C_\mu'' + C_{v_\parallel}'' \otimes I_\mu, \quad (8.18)$$

where $I_{v_{\parallel}} \in \mathbb{R}^{N_{v_{\parallel}} \times N_{v_{\parallel}}}$ and $I_{\mu} \in \mathbb{R}^{N_{\mu} \times N_{\mu}}$ denote identity matrices. The matrix C_{test} has dimension $N_{\mu}N_{v_{\parallel}} \times N_{\mu}N_{v_{\parallel}}$ and is block-tridiagonal, with nine non-zero bands and upper and lower bandwidth $w = N_{\mu} + 1$. The choice to operate on h^T yields a bandwidth $w = N_{\mu} + 1$, whereas an operator that acts on h^T results in a bandwidth $w = N_{v_{\parallel}} + 1$. Since typically in **stella** the number of $v_{\parallel}$ -grid points exceeds the number of μ -grid points, we chose to operate on h^T to obtain a lower bandwidth. The structure of the matrix is shown in Figure 8.1, for $N_{\mu} = 4$ and $N_{v_{\parallel}} = 8$. In **stella**'s collision model, sub-diagonal blocks, associated with the $v_{\parallel,i-1}$ index, are stored in the array **aa_blcs**, on-diagonal and super-diagonal blocks associated with $v_{\parallel,i}$ and $v_{\parallel,i+1}$ are stored in **bb_blcs** and **cc_blcs**, respectively. Individual blocks describe the μ -discretisation, and are tridiagonal. The matrix C_{test} is stored in a compact band format, elements outside the bandwidth of C_{test} are not stored to reduce memory usage.

8.1.2 GAUSS-LAGUERRE GRID

stella provides the option of employing a μ -grid determined by Gauss-Laguerre quadrature. This grid has a non-uniform resolution that increases near the boundary $\mu = 0$. On this non-uniform grid, the two-point centered difference formula employed previously is only first-order accurate. A second-order accurate finite difference scheme for the first derivative on a non-uniform grid is given by the three-point formula (cf. Kálnay de Rivas, 1972)

$$\begin{aligned} \left(\frac{\partial h}{\partial x} \right)_i &\approx \frac{1}{\Delta_{i-1} + \Delta_i} \left[\frac{\Delta_{i-1}}{\Delta_i} h_{i+1} + \frac{\Delta_i^2 - \Delta_{i-1}^2}{\Delta_{i-1} \Delta_i} h_i - \frac{\Delta_i}{\Delta_{i-1}} h_{i-1} \right] \\ &= \frac{1}{\Delta_{i-1} + \Delta_i} \left[\frac{\Delta_{i-1}}{\Delta_i} h'_{i+1/2} + \frac{\Delta_i}{\Delta_{i-1}} h'_{i-1/2} \right], \end{aligned} \quad (8.19)$$

where $h'_{i+1/2} \approx (h_{i+1} - h_i)/\Delta_i$ with $\Delta_i = x_{i+1} - x_i$ and analogously for $h'_{i-1/2}$. Eq. (8.19) resembles the weighted average of the centered differences at the half-indices $i + 1/2$ and $i - 1/2$. We obtain a three-point scheme for the term

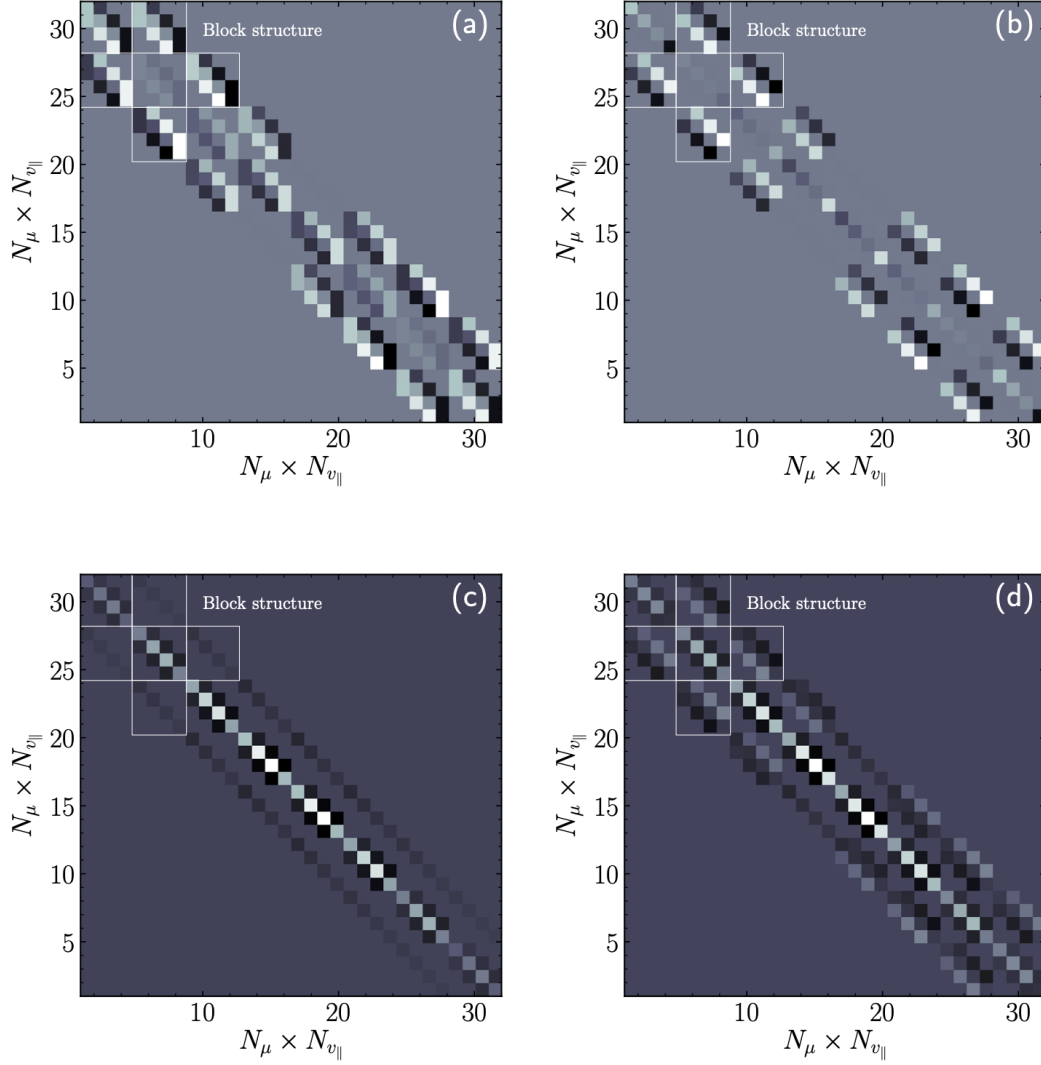


Figure 8.1: Structure of the discretisation matrix of the test particle operator, for $(N_\mu = 4, N_{v_\parallel} = 8)$. (a) Mixed-derivative $C_{v_\parallel\mu}$ -term only, (b) both mixed-derivative terms together are symmetric (c) single-variable terms only (d) combined, symmetric blockmatrix C_{test} . Blocks have dimension $N_\mu \times N_\mu$ and are tridiagonal. The matrix has upper and lower bandwidth $w = N_\mu + 1$, elements outside the band-width vanish. Terms and maximum velocities were rescaled to emphasise the structure of the matrix.

of the form $\partial/\partial x(G\partial h/\partial x)$ by identifying the outer indices in (8.19) with half-

indices whence

$$\frac{\partial}{\partial x} \left[G(x) \frac{\partial h}{\partial x} \right]_i \approx \frac{2}{\Delta_{i-1} + \Delta_i} \left[\frac{\Delta_{i-1}}{\Delta_i} (Gh')_{i+1/2} + \frac{\Delta_i^2 - \Delta_{i-1}^2}{\Delta_{i-1} \Delta_i} (Gh')_i - \frac{\Delta_i}{\Delta_{i-1}} (Gh')_{i-1/2} \right] \quad (8.20)$$

where $h'_{i+1/2} = (h_{i+1} - h_i)/\Delta_i$, analogously for $h'_{i-1/2}$, $G_{i\pm 1/2}$ is evaluated on half-indices and h'_i is approximated using the scheme (8.19). The discretisation (8.20) is used to approximate the single-variable μ -derivative terms in the test particle operator if the Gauss-Laguerre grid is employed.

To approximate the μ -derivatives occurring in the mixed derivative terms in Eq. (7.78) we use the scheme given by (8.19); $v_{\parallel}$ -derivatives on the uniform $v_{\parallel}$ grid are discretised using the standard centered difference. The discretisation of the test-particle operator on the non-uniform μ -grid thus obtained does not ensure exact self-adjointness and density conservation of the test-particle operator. We show in Section 8.3 how exact density conservation can be ensured on a non-uniform grid in the present implementation of the collision operator, and examine the entropy production in Section 9.3. Both exact density conservation and exact self-adjointness can, in principle, be obtained on non-uniform grids by using a discretisation scheme that includes the integration weights (Barnes et al., 2009).

8.2 TIME ADVANCE

The diffusive terms in the test particle operator result in a Courant-Friedrichs-Levy (CFL) timestep constraint that scales with the square of the velocity discretisation size if an explicit time advance scheme is used. Even for a modest collisionality, this can be impractical. To avoid this constraint, the collision operator is implemented in `stella` using an implicit time advance scheme. We make use of Godunov splitting to separate the collisional time

advance from the remainder of the gyrokinetic equation (cf. Barnes et al., 2009). Using the backward Euler method one obtains

$$\frac{g_s^{n+1} - g_s^*}{\Delta t} = C_{\text{GK}}[h_s^{n+1}] = C_{\text{test}}[h_s^{n+1}] + C_{\text{field}}[h_s^{n+1}, h_{s'}^{n+1}] \quad (8.21)$$

where s denotes the species index, g_s^* denotes the distribution function after advancing the non-collisional part of the gyrokinetic equation, and h_s^{n+1} denotes the distribution function after the collisional time advance. In Eq. (8.21), the test-particle operator, $C_{\text{test}}[h_s^{n+1}]$, contains self-collisions and inter-species collisions, but acts only on h_s ; the contributions are therefore collected into a single operator. The field-particle operator acts on h_s and all other species $h_{s'}$. With $g_s^{n+1} = h_s^{n+1} + q_s/T_s J_0 \phi^{n+1} F_{0s}$ it follows that the equation for the species h_s is

$$(1 - \Delta t C_{\text{test}}) h_s^{n+1} = g_s^* + \frac{q_s}{T_s} J_0 \phi^{n+1} F_{0s} + \Delta t C_{\text{field}}[h_s^{n+1}, h_{s'}^{n+1}]. \quad (8.22)$$

Note that we have suppressed spectral indices, and used that the gyroaverage of the electrostatic potential is simply $J_0(k_\perp v_\perp / \Omega) \phi_{\mathbf{k}_\perp}$ in Fourier space. Eq. (8.22) is linear in h_s and can be split into a homogeneous and inhomogeneous component

$$(1 - \Delta t C_{\text{test}}) h_{s,inh}^{n+1} = g_s^* \quad (8.23)$$

$$(1 - \Delta t C_{\text{test}}) h_{s,hom}^{n+1} = \frac{q_s \phi^{n+1}}{T_s} F_{0s} + \Delta t C_{\text{field}}[h_s^{n+1}, h_{s'}^{n+1}], \quad (8.24)$$

with $h_s = h_{s,hom} + h_{s,inh}$. The first, inhomogeneous equation – so called because the right-hand-side depends on the intermediate timestep – can be solved for $h_{s,inh}^{n+1}$ by LU-factorisation of $R = 1 - \Delta t C_{\text{test}}$ and backsubstitution. We use LAPACK's (Anderson et al., 1999) `zgbtrs` algorithm for banded matrices to perform the LU-factorisation of R .

The second, homogeneous equation depends only on quantities at the new timestep $n+1$ and includes the field associated with the electrostatic potential

and an additional field for every term in the Hirshman-Sigmar expansion of the field particle operator. Eq. (8.24) is solved using a Green's function method. We supply a unit impulse to the electrostatic potential and solve $[1 - \Delta t C_{\text{test}}] h_{s, \text{hom}} = q_s J_0 F_{0s} / T_s$ to obtain the response $\delta h_{s, \text{hom}} / \delta \phi$; analogously for each field ψ_j^{lm} appearing in the field-particle operator in Eq. (8.24), we solve $[1 - \Delta t C_{\text{test}}] h_{s, \text{hom}} = \Delta t P_{lm} J_m \Delta_j^{(lm)}$ for the response $\delta h_{s, \text{hom}} / \delta \psi_j^{lm, ss'}$, where we have subsumed multiplicative constants from the field-particle operator into $\Delta_j^{(lm)}$ for clarity. Here all quantities are understood to be at the timestep $n + 1$. Then

$$h_{s, \text{hom}}^{n+1} = \phi^{n+1} \frac{\delta h_{s, \text{hom}}}{\delta \phi} + \sum_{jlm, s'} \psi_{j, lm}^{ss', n+1} \frac{\delta h_{s, \text{hom}}}{\delta \psi_{j, lm}^{ss'}}, \quad (8.25)$$

as can be verified by operating on the equation with $1 - \Delta t C_{\text{test}}$ and where the summation runs over all species, s' , and all j , l and m . The electrostatic potential is related to the distribution function via the quasi-neutrality operator (Barnes et al., 2018)

$$\begin{aligned} \phi = Q[g_s] &:= \frac{1}{\sum_s \frac{Z_s^2}{T_s} (\Gamma_{0s} - 1)} \sum_s Z_s n_s \frac{2B}{\pi^{1/2}} \int J_{0,s} g_s d^3v \\ &= \sum_s Q_s[g_s] \end{aligned} \quad (8.26)$$

where s denotes the species index, $\Gamma_0 := \exp(-k_\perp^2 \rho_s^2 / 2) I_0(k_\perp^2 \rho_s^2 / 2)$, I_0 is the modified Bessel function of the first kind, and we have defined the per-species quasineutrality operator $Q_s[h_s] = \phi_s$ in Eq. (8.26). Operating with Q_s on Eq. (8.25)

$$\phi_{s, \text{hom}}^{n+1} = \phi_s Q_s \left[\frac{\delta h_{s, \text{hom}}}{\delta \phi} \right] + \sum_{jlm, s'} \psi_{j, lm}^{ss', n+1} Q_s \left[\frac{\delta h_{s, \text{hom}}}{\delta \psi_{j, lm}^{ss'}} \right]. \quad (8.27)$$

The fields in the field particle operator are obtained via

$$\psi_{j, lm}^{ss'} = P_{j, lm}^{ss'}[h_{s'}] := c_{l, -m} (-1)^m \int P_{l, -m} J_m h_{s'} \Delta_j^{l, s's} \left(x_s^l L_j^{(l+\frac{1}{2})} (x_s^2) F_{0s} \right) d^3v \quad (8.28)$$

where we have defined the integral operator $P_{j,lm}^{ss'}$ and the Legendre polynomials P_{lm} and constant c_{lm} are defined as in Section 7.3. Operating with $P_{j,lm}^{s's}$ on Eq. (8.25) we obtain

$$\psi_{j,lm,hom}^{s's,n+1} = \phi^{n+1} P_{j,lm}^{s's} \left[\frac{\delta h_{s,hom}}{\delta \phi} \right] + \sum_{ipq,s''} \psi_{i,pq}^{ss'',n+1} P_{j,lm}^{s's} \left[\frac{\delta h_{s,hom}}{\delta \psi_{i,pq}^{ss''}} \right]. \quad (8.29)$$

With $h_{s,inh}^{n+1}$ known from solving the inhomogeneous Eq. (8.23), $\phi_{inh}^s = Q_s[h_{s,inh}]$ and $\psi_{j,lm,inh}^{s's} = P_{j,lm}^{s's}[h_{s,inh}]$ we obtain a linear system of equations for the potential $\phi^{n+1} = \sum_s (\phi_{s,inh}^{n+1} + \phi_{hom}^{s,n+1})$ and the fields $\psi_{j,lm}^{ss',n+1}$ at the new timestep $n+1$, given by

$$[\mathbf{I} - \mathbf{R}] \mathbf{f}^{n+1} = \mathbf{f}_{inh}^{n+1} \quad (8.30)$$

where $\mathbf{f}^{n+1} = [\phi^{n+1}, \{\psi_{j,lm}^{ss',n+1}\}]^T$, $\mathbf{f}_{inh}^{n+1} = [\phi_{inh}^{n+1}, \{\psi_{j,lm,inh}^{ss',n+1}\}]^T$ and $\mathbf{I}$ is the identity matrix. For the case of two species s and s' , the matrix $\mathbf{R}$ is given by

$$\begin{bmatrix} Q[\delta h^\phi] & Q_s[\delta h_s^{\psi_{jlm}^{ss}}] & Q_s[\delta h_s^{\psi_{jlm}^{ss'}}] & Q_{s'}[\delta h_{s'}^{\psi_{jlm}^{s's}}] & Q_{s'}[\delta h_{s'}^{\psi_{jlm}^{s's'}}] & \dots \\ P_{jlm}^{ss}[\delta h_s^\phi] & P_{jlm}^{ss}[\delta h_s^{\psi_{jlm}^{ss}}] & P_{jlm}^{ss}[\delta h_s^{\psi_{jlm}^{ss'}}] & 0 & 0 & \\ P_{jlm}^{ss'}[\delta h_{s'}^\phi] & P_{jlm}^{ss'}[\delta h_s^{\psi_{jlm}^{ss}}] & P_{jlm}^{ss'}[\delta h_s^{\psi_{jlm}^{ss'}}] & 0 & 0 & \\ P_{jlm}^{s's}[\delta h_s^\phi] & 0 & 0 & P_{jlm}^{s's}[\delta h_{s'}^{\psi_{jlm}^{s's}}] & P_{jlm}^{s's}[\delta h_{s'}^{\psi_{jlm}^{s's'}}] & \\ P_{jlm}^{s's'}[\delta h_{s'}^\phi] & 0 & 0 & P_{jlm}^{s's'}[\delta h_{s'}^{\psi_{jlm}^{s's}}] & P_{jlm}^{s's'}[\delta h_{s'}^{\psi_{jlm}^{s's'}}] & \\ \vdots & & & & & \ddots \end{bmatrix} \quad (8.31)$$

where we have used the shorthand $\delta h_s^{\psi_{jlm}^{ss}} := \delta h_s / \delta \psi_{jlm}^{ss}$ for the responses, and for brevity the matrix above shows only one combination of the indices j, l and

m . The response matrix $\mathbf{R}$ has dimension $(1 + N_j N_l^2) \times (1 + N_j N_l^2)$. The LU -factorisation of $\mathbf{R}$ is pre-computed at code initialisation, since all quantities occurring in the response matrix are time-independent.

The linear system (8.30) can then be solved for the fields $\{\phi^{n+1}, \psi_{j,lm}^{ss',n+1}\}$ at every timestep by backsubstitution. With the fields $\{\phi^{n+1}, \psi_{j,lm}^{ss',n+1}\}$ computed, the implicit time advance equation (8.22) is solved for the distribution function at the new timestep, h^{n+1} . The functions $\Delta_j^{ss',l}$ in the field particle operator are computed during code initialisation, using recursive functions that implement Eq. (7.36) based on the operator $C_v^{ab} =: \Delta_0^{ab}$. A pseudocode description of the collision algorithm in `stella` is shown in Section 8.2.1.

8.2.1 OVERVIEW OF THE stella COLLISION ALGORITHM

Algorithm 1 Pseudocode of the `stella` collision algorithm

Initialisation:

```

1: Initialise non-collisional code
2: if Collisions then
3:   Initialise collision frequencies ▷ init_nusDpa
4:   Initialise test particle operator ▷ init_fp_diffmatrix
5:   if Field Particle Operator then
6:     Initialise  $\Delta_j^{ls}$  ▷ init_deltaaj_vmu
7:   end if
8:   Compute response matrix  $\mathbf{R}$ ,  $LU$ -decompose ▷ init_fp_conserve
9: end if
```

Time advance loop:

```

10: while  $n < N_{\text{timestep}}$  do
11:   Non-collisional advance from  $g^n$  to  $g^*$ 
12:   if Collisions then ▷ advance_implicit_fp
13:     Solve  $(I - C_{\text{test}})h_{inh}^{n+1} = g^*$  ▷ Band-matrix algorithm zgbtrs
14:     Compute  $\phi_{inh}^{n+1} = Q[h_{inh}^{n+1}]$  ▷ get_fields
15:     if Field Particle Operator then
16:       Compute  $\psi_{inh,jlm}^{ss',n+1} = P_{jlm}^{ss'}[h_{s,inh}^{n+1}]$  ▷ get_psi
17:       Solve Eq. (8.30) for  $\phi^{n+1}, \psi_{jlm}^{ss',n+1}$  ▷ lu_back_substitution
18:       Get RHS of implicit Euler Eq. (8.22) with  $\phi^{n+1}, \psi_{jlm}^{ss',n+1}$ 
19:     end if
20:     Solve implicit Euler Eq. (8.22) for  $h^{n+1}$  ▷ zgbtrs
21:     Get  $g^{n+1}$  from  $h^{n+1}$ 
22:   end if
23:    $n \leftarrow n + 1$ 
24: end while
```

8.3 CONSERVATION PROPERTIES

8.3.1 EXACT DENSITY CONSERVATION ON NON-UNIFORM GRIDS

It can be shown that the first two terms in the field-particle operator expansion correspond to energy and momentum conserving operators that compensate the energy and momentum production of the test particle operator to ensure overall conservation (cf. Hirshman and Sigmar, 1976; Abel et al., 2008). To guarantee the conservation of density, momentum and energy to machine precision, care must be taken in performing the discretisation of the test particle operator and the integrals in the field particle operator. Density conservation of the test particle operator is guaranteed automatically if the uniform velocity grid and uniform integration weights are employed (cf. Section 8.1). In the case of the μ -grid chosen by Gauss-Laguerre quadrature, the density moment of the test-particle operator vanishes only approximately, and density conservation is dependent on the velocity space resolution. We can enforce exact conservation of density by the collision operator by introducing an additional term in the field particle operator, $F_{0s}^* \psi_{j=0}^{s,l=0,*}$, with

$$F_{0s}^* \psi_{j=0}^{s,l=0,*} = F_{0s}^* \frac{\int \sum_{s'} C_{\text{test}}^{ss'}[h_{s'}] d^3v}{\int F_{0s}^* d^3v}, \quad (8.32)$$

where the sum over s' accounts for contributions from like-species and inter-species collisions. The numerator in (8.32) is the total density of species s produced artificially in collisions with species s' . Since the density moment of the test-particle operator calculated numerically is approximately zero, the term $F_{0s}^* \psi_{j=0}^{s,l=0,*}$ is a small correction to the collision operator. The function F_{0s}^* must be chosen so that momentum and energy conservation of the total collision operator remain intact. With

$$F_{0s}^* = F_{0s} - v^2 F_{0s} \frac{\int v^2 F_{0s} d^3v}{\int v^4 F_{0s} d^3v} \quad (8.33)$$

where F_{0s} is the Maxwellian, this is guaranteed since the parallel momentum and energy moments of F_{0s}^* vanish, independent of the numerical integration scheme if integrals are calculated consistently using the same numerical scheme. With the addition of the term (8.32) to the field-particle operator, we have enforced exact density conservation of the collision operator on unequally spaced velocity grids.

Density conservation of the field particle operator is automatically satisfied for terms in the operator that are odd in $v_{\parallel}$, since **stella** employs a grid for integration in $v_{\parallel}$ that is anti-symmetric around $v_{\parallel} = 0$. For even terms, exact density conservation is not guaranteed. To enforce this, for the energy restoring term $\{l = 0, j = 1\}$, we make the modification

$$\Delta_{j=1}^{l,ss'} \mapsto \Delta_{j=1}^{l,ss'} - \frac{F_{0s}^*}{\int F_{0s}^* d^3v} \int \Delta_{j=1}^{l,ss'} d^3v, \quad (8.34)$$

to ensure conservation of number density to machine precision. The modification (8.34) remains accurate as long as the integral over $\Delta_{j=1}^{l,ss'}$ is small; in numerical tests the modification incurs at worst a 10% error, in the case of disparate mass ratios $\mu \leq 10^{-4}$ at the default velocity space resolution.

8.3.2 EXACT MOMENTUM AND ENERGY CONSERVATION

Interspecies momentum conservation requires that for $k_{\perp} = 0$

$$\int m_s v_{\parallel} C_{\text{test}}^{ss'}[h_s] d^3v = - \int m_{s'} v_{\parallel} C_{\text{field}}^{s's}[h_s] d^3v. \quad (8.35)$$

Using $P_{l=1}^{m=0}(\cos \theta) = v_{\parallel}/v$, the self-adjointness of $\Delta_j^{ss'}$ and $\int v_{\parallel}^2/v^2 f(v) d^3v = \int \cos^2(\theta) \sin \theta d\theta \int f(v) v^2 dv = 2/3 \int f(v) v^2 dv = \frac{1}{3} \int f(v) d^3v$ on the right-hand side, one obtains

$$\int m_s v_{\parallel} C_{\text{test}}^{ss'}[h_s] d^3v = -m_{s'} \int \frac{h_s}{F_{0s}} \frac{v_{\parallel}}{v} \Delta_{j=0}^{l=1,ss'}[v F_{0s'}] d^3v. \quad (8.36)$$

For this condition to be satisfied to machine precision we use that $\Delta_{j=0}^{ss',l=1}$ can be expressed using the test-particle operator. A straightforward calculation shows that

$$\Delta_{j=0}^{ss',l=1}[x_{s'} \exp(-x_{s'}^2)] = \mu_{ss'}^2 x_s \nu_s^{ss'}(x_s) \exp(-x_s^2) \quad (8.37)$$

where ν_s is the slowing-down frequency from the test particle operator. Using the identity (8.37) and the differential identities from Abel et al. (2008) yields

$$\frac{v_{\parallel}}{v} \Delta_{j=0}^{ss',l=1}(x_{s'} F_{0s'}) = \frac{1}{v_{th,s}} \frac{m_s}{m_{s'}} C_{\text{test}}^{ss'}[v_{\parallel} F_{0s}]. \quad (8.38)$$

We can compute $\Delta_{j=0}^{l=1,ss'}$ using (8.38) in the numerical implementation of the field particle operator. Exact momentum conservation (8.35) is then guaranteed so long as the test-particle operator satisfies exact self-adjointness, which is the case if uniform velocity grids are employed. To ensure exact momentum conservation on non-uniform velocity grids, we can replace the field particle term with the integral moment of the test particle operator using (8.35). This comes at an additional computational cost since the test-particle operator acting on h_s in (8.35) must be evaluated before the integral is computed.

Energy conservation is treated analogously. Conservation to machine precision requires

$$\int m_s v^2 C_{\text{test}}^{ss'}[h_s] d^3v = - \int m_{s'} v^2 C_{\text{field}}^{s's}[h_s] d^3v. \quad (8.39)$$

Writing out the $\Delta_{j=1}^{ss',l=0}$ -term of the field particle operator on the right-hand-side gives

$$\int m_s v^2 C_{\text{test}}^{ss'}[h_s] d^3v = m_{s'} \int \frac{h_s}{F_{0s}} \Delta_{j=1}^{ss',l=0}[(3/2 - x_{s'}^2) F_{0s'}] d^3v. \quad (8.40)$$

Relating $\Delta_{j=1}^{ss',l=0}$ to the collision frequencies occurring in the test particle operator yields

$$\Delta_{j=1}^{ss',l=0}[(3/2 - x_{s'}^2) \exp(-x_{s'}^2)] = -\mu_{ss'}^{3/2} x_s^2 \nu_E^{ss'}(x_s) \exp(-x_s^2). \quad (8.41)$$

Again using the differential identities of Abel et al. (2008) for the collision frequencies occurring in the test-particle operator it follows that

$$\Delta_{j=1}^{ss',l=0}[(3/2 - x_{s'}^2)F_{0s'}] = C_{\text{test}}^{ss'}[m_s v^2 F_{0s}]. \quad (8.42)$$

We can use (8.42) to calculate $\Delta_{j=1}^{ss',l=0}$ using the test-particle operator. Exact conservation of energy is then ensured if the test-particle operator satisfies exact self-adjointness. On non-uniform grids, where this is not the case, we use (8.39) directly to evaluate the energy-conserving term in the field-particle operator, at the additional computational expense of calculating the test particle operator acting on h_s .

CHAPTER 9

TESTS AND BENCHMARKS

In this chapter, we subject the collision model implemented in `stella` to a number of tests and perform benchmarks against the collision model of the gyrokinetic code `GS2`. We also demonstrate the superior accuracy of the collision model by solving the Spitzer problem and perform initial collisional gyrokinetic simulations.

9.1 BENCHMARK AGAINST GS2

We begin by testing the implementation of the test-particle operator through a benchmark against the test-particle operator implemented in the gyrokinetic solver `GS2` (Kotschenreuther et al., 1995). The `GS2` collision model is described in detail in Barnes et al. (2009) and Abel et al. (2008); we briefly recapitulate key features here: the code uses (E, λ) -velocity space coordinates, where E denotes the particle kinetic energy, and $\lambda = \mu/E$, with μ denoting the magnetic moment. The test-particle operator implemented in `GS2` is the pitch-angle scattering and energy diffusion test-particle operator described in Section 7.2. The field particle operator implemented in `GS2` consists of two terms that ensure conservation of momentum and energy by the full collision operator.

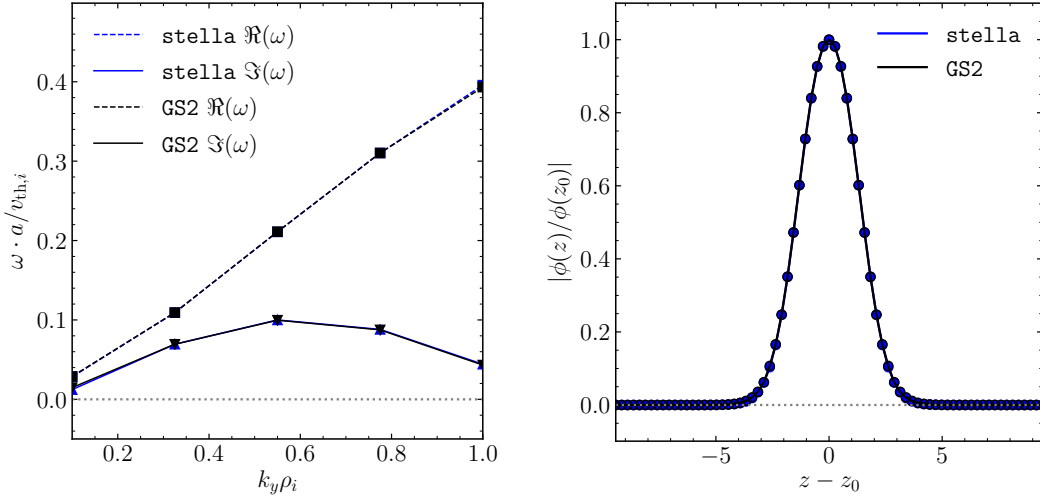


Figure 9.1: *Left*: Growth rates (solid lines) and real frequencies (dashed lines) for a collisionless ($\nu_{ii}a/v_{th,i} = 0.0$) Cyclone Base Case simulation, with **GS2** (black) and **stella** (blue). *Right*: Electrostatic potential for the fastest growing mode ($k_y \rho_i = 0.55$) as a function of the parallel coordinate.

The energy-conserving term corresponds exactly to the $\{j = 1, l = 0\}$ -energy-conserving term of the collision model introduced here, and is given by (Barnes et al., 2009)

$$E[h_{\mathbf{k}}] = v^2 \nu_E J_0(a) F_0 \frac{\int \nu_E v^2 J_0(a) h_{\mathbf{k}} d^3 v}{\int \nu_E v^4 F_0 d^3 v}. \quad (9.1)$$

where $a := k_{\perp} v_{\perp} / \Omega$ and species indices have been suppressed everywhere. The momentum conserving term implemented in **GS2** differs from the momentum conserving term implemented in **stella**. The Lorentz and energy diffusion operators in **GS2** are implemented using an operator-splitting method; to ensure exact momentum conservation of each operator while retaining self-adjointness, the Lorentz operator is combined with a momentum conserving term given by (Barnes et al., 2009)

$$U_L[h_{\mathbf{k}}] = \nu_D F_0 \left[J_0(a) v_{\parallel} \frac{\int \nu_D v_{\parallel} J_0(a) h_{\mathbf{k}} d^3 v}{\int \nu_D v_{\parallel}^2 F_0 d^3 v} + J_1(a) v_{\perp} \frac{\int \nu_D v_{\perp} J_1(a) h_{\mathbf{k}} d^3 v}{\int \nu_D v_{\perp}^2 F_0 d^3 v} \right]. \quad (9.2)$$

while momentum conservation for the energy diffusion term is ensured with the operator

$$U_D[h_{\mathbf{k}}] = -\Delta\nu F_0 \left[J_0(a)v_{\parallel} \frac{\int \Delta\nu v_{\parallel} J_0(a) h_{\mathbf{k}} d^3v}{\int \Delta\nu v_{\parallel}^2 F_0 d^3v} + J_1(a)v_{\perp} \frac{\int \Delta\nu v_{\perp} J_1(a) h_{\mathbf{k}} d^3v}{\int \Delta\nu v_{\perp}^2 F_0 d^3v} \right]. \quad (9.3)$$

Here the collision frequency $\Delta\nu := \nu_D - \nu_s$. The momentum conserving terms given by Eqs. (9.2) and (9.3) are a modification of the momentum conserving term provided in Abel et al. (2008), given by

$$U[h_{\mathbf{k}}] = \nu_s F_0 \left[J_0(a)v_{\parallel} \frac{\int \nu_s v_{\parallel} J_0(a) h_{\mathbf{k}} d^3v}{\int \nu_s v_{\parallel}^2 F_0 d^3v} + J_1(a)v_{\perp} \frac{\int \nu_s v_{\perp} J_1(a) h_{\mathbf{k}} d^3v}{\int \nu_s v_{\perp}^2 F_0 d^3v} \right]. \quad (9.4)$$

The momentum conserving term given by Eq. (9.4) is identical to the momentum conserving term implemented in **stella**. With this in mind, we performed benchmark gyrokinetic simulations to test if the energy and momentum conserving terms of the field particle operator in **stella** reproduce results obtained with **GS2**.

9.1.1 CYCLONE BASE CASE SIMULATIONS

Linear gyrokinetic simulations of the Cyclone Base Case (CBC) regime of the DIII-D tokamak (Dimits et al., 2000), a commonly used test-case for gyrokinetic codes, were first performed to benchmark the test-particle collision operator of **stella** against the operator implemented in **GS2**. The simulations were performed with kinetic ions; electrons were approximated to adiabatically stream along magnetic field lines, so that $\delta n_e = en_{e0}\phi/T_e$. In **stella**, we used 24 grid-points in the field-line following coordinate z , 48 grid-points in $v_{\parallel}$ and 12 points in μ on a Gaussian grid, and evolved the code for 4000 time-steps with $\Delta t = 0.008a/v_{th,i}$. In **GS2**, we used $n_{\lambda} = 33$ grid-points in λ , $n_E = 32$ grid-points in the energy coordinate and 24 grid-points in the field-line following coordinate. The velocity space cut-off speed was set to $v_{\parallel,c} = v_{\perp,c} = 3.0v_{th,s}$ in

stella and $v_c = 3.0v_{th,s}$ in **GS2**. The simulation parameters are summarised in Table 9.1.

Growth rate and frequency spectra obtained with both codes are shown in Figure 9.1, for a non-collisional simulation ($\nu_{ii}a/v_{th,i} = 0$), and in Figure 9.2 for a highly collisional simulation ($\nu_{ii}a/v_{th,i} = 0.1$) that employed only the test-particle operators in both codes. Excellent agreement of the growth rates and frequencies is obtained over the extent of the spectrum in both cases. The inclusion of the test-particle component of the collision operator reduces the growth rates in both codes by 30%, from a maximum normalised growth rate of $\gamma a/v_{th,i} = \text{Im}(\omega)a/v_{th,i} = 0.1$ at a wave number $k_y\rho_i = 0.55$ in the absence of collisions, to $\gamma a/v_{th,i} = 0.07$ at $k_y\rho_i = 0.55$ with strong test-particle collisions enabled. The modest reduction of the ITG growth rate for a high collisionality is consistent with findings that collisions only weakly affect the growth rates of drift waves that are driven by an ion temperature gradient in a toroidal geometry (Kauffmann et al., 2010).

A comparison of the energy-diffusion and energy-conserving terms in **stella** and **GS2** was also performed via a collisional CBC simulation. In **stella**, the Lorentz operator was suppressed in the collision model, and the field-particle operator expansion included only the $\{j = 1, l = 0\}$ -term associated with energy conservation. Analogously the Lorentz operator was disabled in **GS2** and terms associated with perpendicular momentum conservation of the energy diffusion operator were suppressed. The remaining terms in the **GS2** collision operator are then energy diffusion and energy conservation. Growth rates and real frequencies for both codes are shown in Figure 9.3 (left plot), with excellent agreement over the range of wavenumbers.

Figure 9.3 (right plot) shows the frequency and growth rate spectra when the respective momentum conserving terms in the field particle operator are included in **GS2** and **stella**. Good agreement is obtained at low $k_\perp\rho_i$, with a

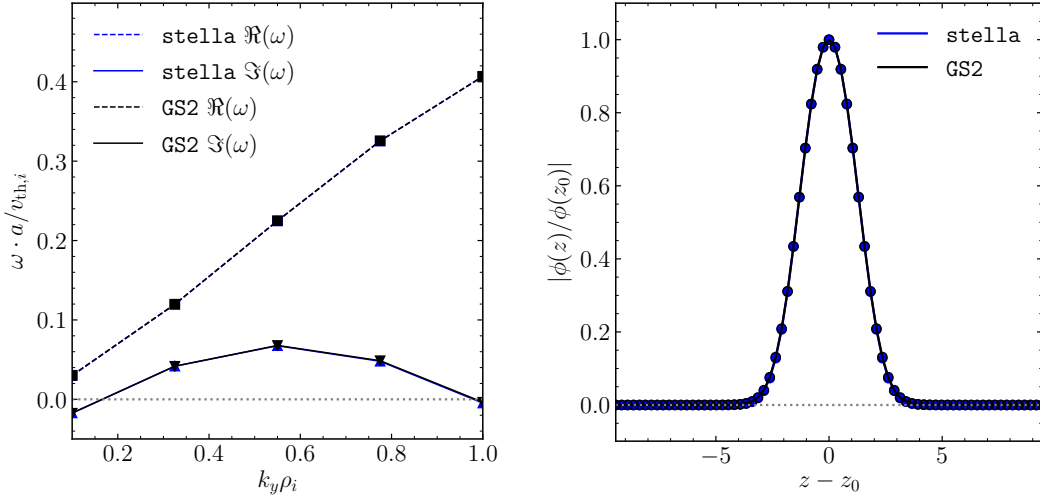


Figure 9.2: *Left:* Growth rates (solid lines) and real frequencies (dashed lines) for a collisional ($\nu_{ii}a/v_{th,i} = 0.1$) Cyclone Base Case simulation, with GS2 (black) and *stella* (blue). Only the test particle operator was included in the collision model. *Right:* Electrostatic potential for the fastest growing mode ($k_y \rho_i = 0.55$) as a function of the parallel coordinate.

small discrepancy at $k_{\perp} \rho_i \sim 1$. We attribute this discrepancy to the modification, made for numerical purposes, of the momentum conserving terms in GS2 described previously. The disagreement is more pronounced at $k_{\perp} \rho_i \sim 1$ because the Bessel function $J_1(a)$, occurring in the perpendicular momentum conserving terms in Eqs. (9.2) and (9.3) are $J_1(a) \sim 1$ for $a \sim 1$ while $J_1(a) \rightarrow 0$ for $a \rightarrow 0$, where the argument of the Bessel function $a = k_{\perp} v_{\perp} / \Omega$. The parallel momentum conserving terms in (9.2) and (9.3) are small for the CBC simulations performed here because the distribution function was approximately symmetric in $v_{\parallel}$; the integrals in the parallel momentum conserving terms, that are odd in $v_{\parallel}$, are then small.

9.1.2 CBC SIMULATION WITH KINETIC ELECTRONS

Simulations of the Cyclone Base Case were also performed with both ion and electron species treated kinetically, to test interspecies collision terms. Be-

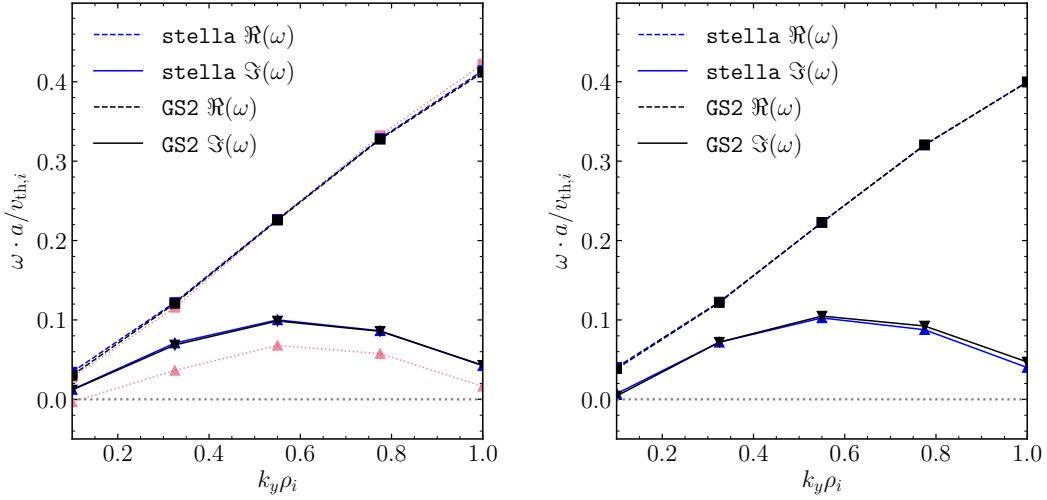


Figure 9.3: *Left*: Growth rates (solid lines) and real frequencies (dashed lines) for a collisional ($\nu_{ii}a/v_{th,i} = 0.1$) Cyclone Base Case simulation with only energy diffusion and energy-conserving terms included in the collision operator, with GS2 (black) and *stella* (blue). Growth rates and frequencies for an energy diffusion operator without the energy-conserving term are shown for comparison (red dotted lines). *Right*: Growth rates and real frequencies for the full test-particle operator and energy and momentum conserving terms in both codes. The small discrepancy at $k_y \rho_i \sim 1$ is associated with the modification of the perpendicular momentum conserving terms made in the collision operator of GS2.

cause the Spitzer collisionality scales with the inverse square root of the species mass, the electron collision frequency exceeds the ion collision frequency by a factor $(m_i/m_e)^{1/2} = 60.6$ for a deuterium plasma; accordingly the simulations were performed with $\nu_{ii}a/v_{th,i} = 0.1$ and $\nu_{ee}a/v_{th,i} = \nu_{ei}a/v_{th,i} = 6.06$. For interspecies collisions, the collision model in GS2 makes use of a mass-ratio expansion to discard ion-electron test-particle collisions and electron-ion energy diffusion; the Lorentz operator is further simplified by utilizing a mass ratio expansion to approximate the electron-ion deflection frequency with $\nu_D^{ei}(v) = \nu_{ei}(v_{th,e}/v)^3$ (cf. Abel et al., 2008; Barnes et al., 2009). A comparison of the growth rates and frequencies obtained with both codes for ion-scale wavenumbers, $k_y \rho_i \lesssim 1$, is shown in Figure 9.4 (left plot), demonstrating very

good agreement between the codes. Growth rates and frequencies on electron scales $k_y \rho_i \lesssim 60$ are shown in Figure 9.4 (right plot), also demonstrating very good agreement throughout the spectrum. These benchmarks give us confidence that the collision model in **stella** performs as expected. We note that while a mass ratio expansion of the collision operator as employed in **GS2** is acceptable for small mass ratios associated with electron-ion collisions, this inevitably is inaccurate for collisions between ion species that have comparable masses, such as Deuterium and Tritium species, a point we return to in the conclusion on possible future work with collisional **stella**.

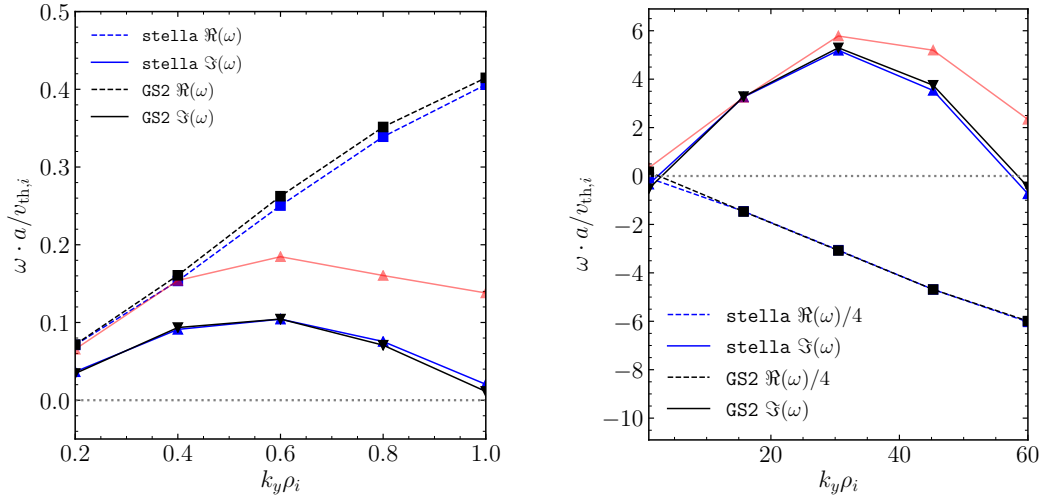


Figure 9.4: *Left:* Growth rates (solid lines) and real frequencies (dashed lines) for a collisional ($\nu_{ii}a/v_{th,i} = 0.1$, $\nu_{ee}a/v_{th,i} = 6.06$) CBC simulation with kinetic ions and electrons, on ion scales. *Right:* Growth rates and real frequencies on electron scales, with growth rates for a non-collisional simulation shown for comparison in red.

9.2 CONSERVATION LAWS

We next examine the conservation properties of the collision model in **stella**. The collision operator should conserve density, momentum and energy. How-

ever, the conversion of the collision operator into the gyrokinetic form introduced spatial dependencies via the gyrodiffusive term and Bessel functions; as a result the first three velocity moments no longer vanish when $k_\perp \neq 0$. Abel et al. (2008) and Barnes et al. (2009) have shown that the conservation laws for the gyrokinetic collision operator can be expressed as a condition on the collision operator in the limit $k_\perp = 0$, namely, requiring

$$\int d^3v (1, v_\parallel, v^2)^T C_{\text{GK}, k_\perp=0}[h_{\mathbf{k}}] = 0 \quad (9.5)$$

ensures that density, momentum and energy are locally conserved by the collision operator (Abel et al., 2008). Here $C_{\text{GK}, k_\perp=0}$ denotes the gyrokinetic collision operator with all finite Larmor radius terms of the operator disabled in both the test and field particle components (cf. Abel et al., 2008). By construction of the collision model implemented in **stella** this condition is satisfied if the $\{j = 1, l = 0\}$ and $\{j = 0, l = 1\}$ terms are retained in the spherical harmonic and Hirshman-Sigmar expansion of the field-particle operator. To test that these conservation properties hold for the numerical implementation of the collision model, the distribution function was initialised with non-zero density, momentum and energy moments as

$$h(v_\parallel, \mu) = \left[1 + \frac{mv_\parallel}{T_0} \delta u_{\parallel,0} + \left(\frac{mv_\parallel^2}{T_0} - \frac{1}{2} \right) \frac{\delta T_{\parallel,0}}{T_0} \right] F_{0s} \quad (9.6)$$

where $\delta u_{\parallel,0}$ and $\delta T_{\parallel,0}$ are constants. All non-collisional terms in the gyrokinetic equation were disabled. The evolution of the density, momentum and energy was then measured over 20 collision times, shown in Figure 9.5, with and without the conserving terms in the collision operator. Density conservation to machine precision was verified for uniform velocity space grids, where the integration weights are equal to the inverse grid spacing. For the μ -grid determined by Gauss-Laguerre quadrature a small density variation $\delta n_i(t)/\delta n_i(t=0) \sim 10^{-3}$ is found; density is only approximately conserved

on this non-uniform grid. Inclusion of the density correction term in the field particle operator introduced in Section 8.3 ensures conservation to machine precision on the non-uniform μ -grid. The parallel momentum decays significantly over 20 collision times in the absence of the field particle operator. Inclusion of the $\{j = 0, l = 1, m = 0\}$ -term in the field particle operator, calculated as prescribed in Section 8.3 leads to parallel momentum conservation to machine precision. Similarly, inclusion of the $\{j = 1, l = 0, m = 0\}$ term ensures that energy is conserved to machine precision. These tests demonstrate that the numerical implementation of the collision model satisfies the conservation laws required for a physical collision operator.

9.3 H-THEOREM

Boltzmann's H-theorem mandates that the entropy production rate of the collision operator must be non-negative at all times and zero if and only if the distribution function is Maxwellian. To verify that this holds, the distribution function was initialised as random in velocity space, with $h(v_{\parallel}, \mu)$ drawn from the uniform distribution $U[-1/2, 1/2]$, following Barnes et al. (2009). The phase-space average of the entropy is given by

$$S = - \int d^3v \int \frac{d^3\mathbf{R}}{V} f \ln f, \quad (9.7)$$

and, expanding the distribution function around a Maxwellian $f = F_0 + \delta f$, to lowest order one obtains

$$S = - \int d^3v \int \frac{d^2\mathbf{R}}{V} \frac{\delta f^2}{2F_0}. \quad (9.8)$$

The time evolution of the rate of change of S , $dS/dT \propto \Delta S = (S_{i+1} - S_i)$ where i denotes the timestep, is shown in Figure 9.6. On the uniform velocity grid, the entropy production rate is always positive and decays uniformly until it reaches machine precision $\sim 10^{-15}$ at $t\nu_{ii} = 80$, as is expected for a

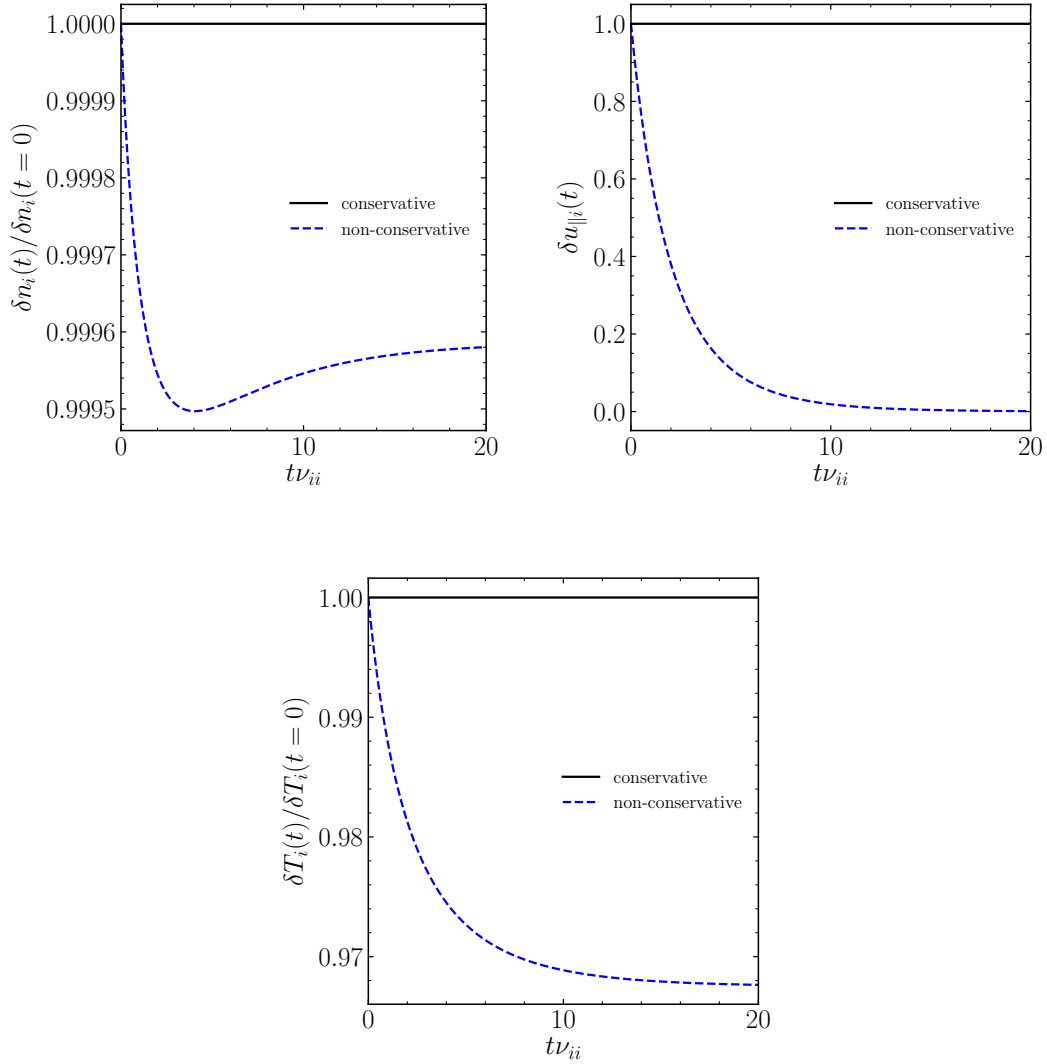


Figure 9.5: Evolution of the perturbed ion density (*top left*), parallel flow (*top right*) and energy (*bottom*) due to the collision model in the limit $k_{\perp} = 0$, over 20 collision times. The distribution function was initialised as defined in Eq. (9.6). Including the density restoring term and the $\{j = 0, l = 1, m = 0\}$ and $\{j = 1, l = 0, m = 0\}$ terms of the field-particle operator ensures conservation of the first three moments to machine precision [continuous black line], when these terms are computed as described in Sec. 8.3.2.

scheme that guarantees exact self-adjointness. On the μ -grid determined by Gauss-Laguerre quadrature, the entropy production rate is positive and decays over thirteen orders of magnitude as the distribution function approaches a

Maxwellian distribution in velocity space. At $\Delta S(t) \approx 10^{-6.5}$ negative entropy production sets in that then decays to $\Delta S(t) \approx 10^{-9}$ at $t\nu_{ii} = 80$. While the H-theorem can therefore be violated on non-uniform velocity grids, such a small deviation is likely benign and can be checked using the uniform velocity grid. Convergence of the distribution function to a Maxwellian was verified by examining the velocity space of the distribution function.

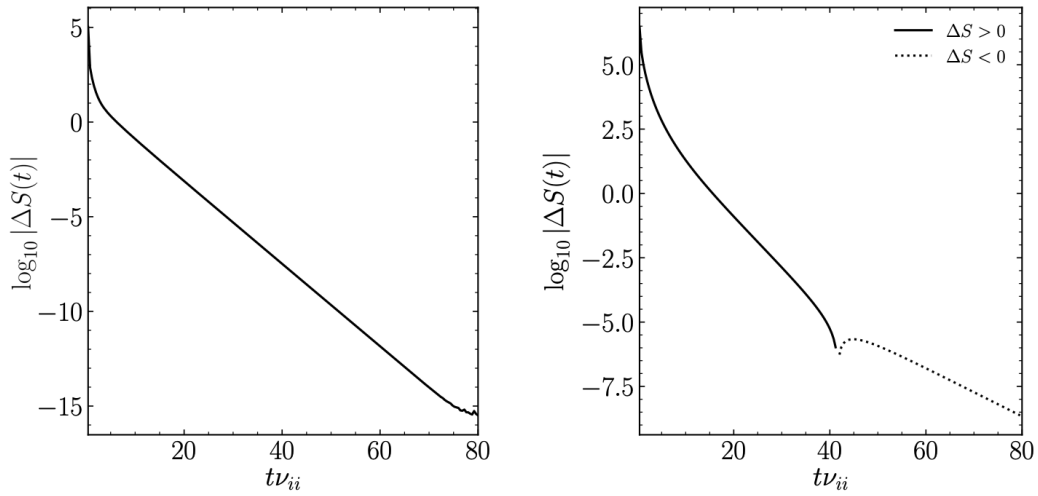


Figure 9.6: Rate of change of the entropy due to collisions. *Left:* entropy production for the numerical scheme that ensures exact self-adjointness of the collision operator on uniform velocity-space grids. The entropy production is always non-negative and approaches zero as the distribution function approaches a Maxwellian. *Right:* entropy production for the Gauss-Laguerre μ -grid on which the collision operator is only approximately self-adjoint. The entropy production is non-negative (solid line) and decays over 14 orders of magnitude as the distribution function approaches a Maxwellian, before small negative entropy production sets in (dotted line) that then decays.

9.4 THE SPITZER PROBLEM

To test the accuracy of the collision model and to demonstrate the utility of the model field-particle operator, we solve the time independent parallel Spitzer

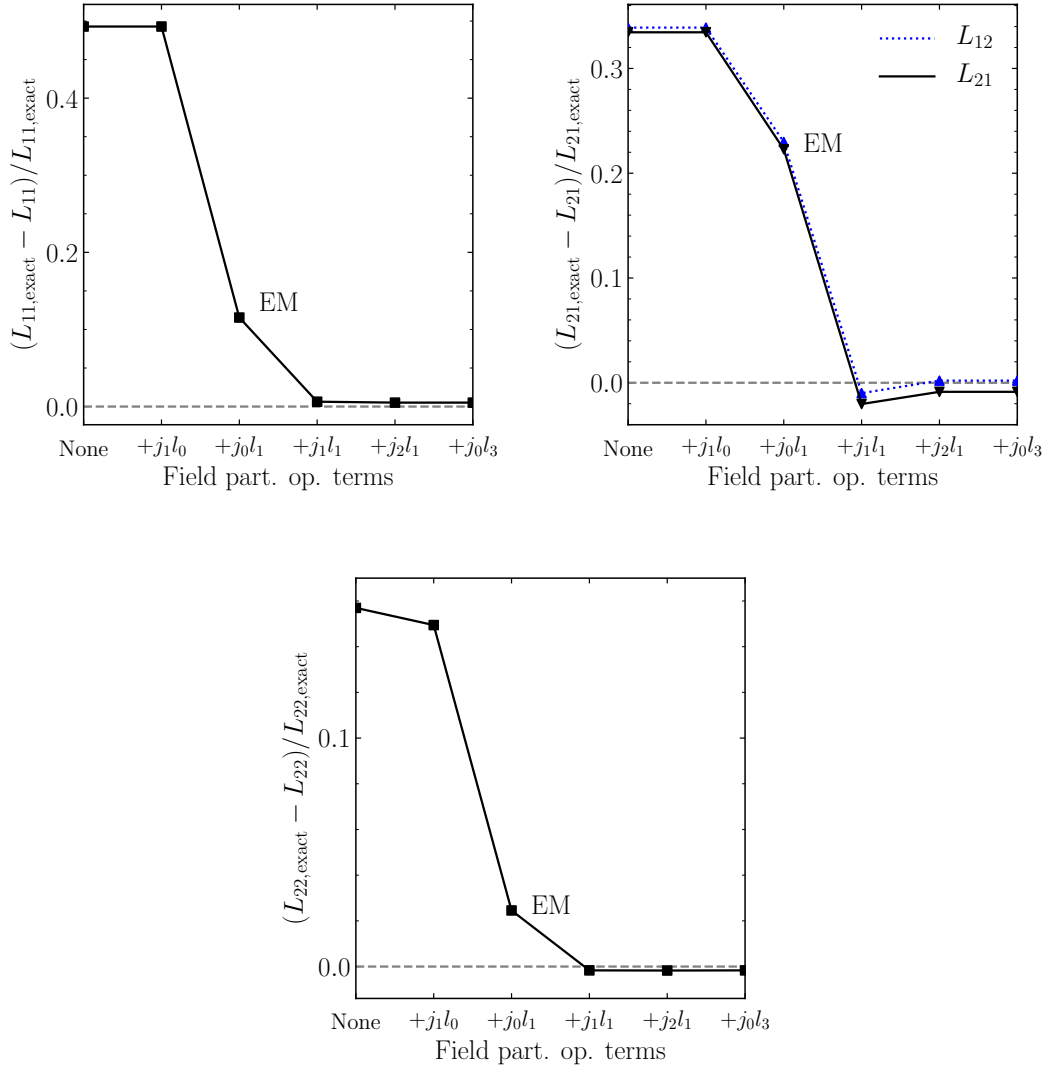


Figure 9.7: Errors in the Spitzer transport coefficients calculated with `stella`, relative to coefficients determined with the exact Fokker-Planck operator by Belli and Candy (2011), for successively added terms in the field particle operator expansion. The energy and momentum conserving collision model (EM) consists of the $\{j = 0, l = 1\}$ and $\{j = 1, l = 0\}$ terms. Including higher-order terms in the field particle operator expansion up to the $\{j = 2, l = 1\}$ term yields errors below 1%. Scans were performed with $N_{v_{\parallel}} = 72$ and $N_{\mu} = 42$ velocity-space grid-points. The center plot shows that $L_{12} \approx L_{21}$, demonstrating Onsager symmetry.

problem. To do so, we disable all non-collisional terms in the gyrokinetic equation, and introduce momentum and energy flux source terms associated with

a constant applied parallel electric field, $E_{\parallel}$, and parallel pressure and temperature gradients, $\nabla_{\parallel} \ln p_{0e}$ and $\nabla_{\parallel} \ln T_{0e}$, respectively. The Spitzer problem then consists in solving

$$C_{ee}[f_e] + C_{ei}[f_e, f_{0i}] = - \left[v_{\parallel} \underbrace{\left(\frac{q_e E_{\parallel}}{T_e} - \nabla_{\parallel} \ln p_{0e} \right)}_{=: I_1} + v_{\parallel} \left(x_e^2 - \frac{5}{2} \right) \underbrace{[-\nabla_{\parallel} \ln T_{0e}]}_{=: I_2} \right] F_{0e}. \quad (9.9)$$

for the electron distribution function, where we have defined the thermodynamic forces $I_1 := q_e E_{\parallel} / T_e - \nabla_{\parallel} \ln p_{0e}$ and $I_2 := -\nabla_{\parallel} \ln T_{0e}$. To implement the time independent Spitzer problem in **stella** we take a single timestep that is large relative to the collision time, so that $\tau_c / \Delta t \rightarrow 0$. The linearity of Eq. (9.9) implies that the particle and heat fluxes can be written as linear combinations of the thermodynamic forces (cf. Helander and Sigmar, 2002)

$$\frac{4m_e \tau_{ei}^{-1}}{3\sqrt{\pi} n_{0e} T_{0e}} \int d^3v v_{\parallel} f_e = L_{11} I_1 + L_{21} I_2 \quad (9.10)$$

and

$$\frac{4m_e \tau_{ei}^{-1}}{3\sqrt{\pi} n_{0e} T_{0e}} \int d^3v v_{\parallel} \left(x_e^2 - \frac{5}{2} \right) f_e = L_{12} I_1 + L_{22} I_2, \quad (9.11)$$

where the coefficients L_{11} , L_{12} , L_{21} and L_{22} denote the Spitzer coefficients (cf. Helander and Sigmar, 2002; Belli and Candy, 2011), and

$$\tau_{ei}^{-1} = \frac{\sqrt{2\pi} q_e^2 q_i^2 n_{0i} \ln \Lambda}{m_e^{1/2} T_{0e}^{3/2}}. \quad (9.12)$$

To evaluate the accuracy of the collision model in **stella**, scans were performed in the Spitzer coefficients over the number of terms included in the field particle operator collision model. These scans employed the non-uniform velocity space grid in **stella** for better accuracy of the numerical integrals. Residuals were calculated with respect to Spitzer coefficients computed using the exact Fokker-Planck operator (Belli and Candy, 2011), implemented in

the neoclassical solver **NEO** (Belli and Candy, 2008). The residuals are shown in Figure 9.7. Retaining only the first two terms in the expansion of the field particle operator ($\{l = 0, j = 1\}, \{j = 1, l = 0\}$) – corresponding to the energy and momentum conserving collision model commonly used in gyrokinetic codes such as **GS2** – yields errors of $\sim 10\% - 25\%$. Additionally including the $\{j = 1, l = 1\}$ term associated with the collisional energy flux density reduces the errors in all three coefficients to $1\% - 5\%$; adding higher-order terms up to $\{j = 2, l = 1\}$ results in errors below 1% in all three coefficients. In performing these scans, all m -indices associated with an l -index were included. The Spitzer coefficients L_{12} and L_{21} exhibit an important symmetry $L_{12} = L_{21}$, known as Onsager symmetry (Onsager, 1931). It can be shown that Onsager symmetry is a consequence of the self-adjointness of the collision operator. By design of the approximate collision model used here, self-adjointness holds term by term in the expansion of the field particle operator; indeed, a comparison of L_{12} and L_{21} in Figure 9.7 for an increasing number of terms in the field particle operator expansion confirms that Onsager symmetry holds, if only approximately, for the collision model when non-uniform velocity-space grids are employed. The scans performed in the Spitzer coefficients demonstrate that the accuracy of the collision model implemented in **stella** can indeed be increased progressively and rigorously approximates the exact linearised Fokker-Planck operator.

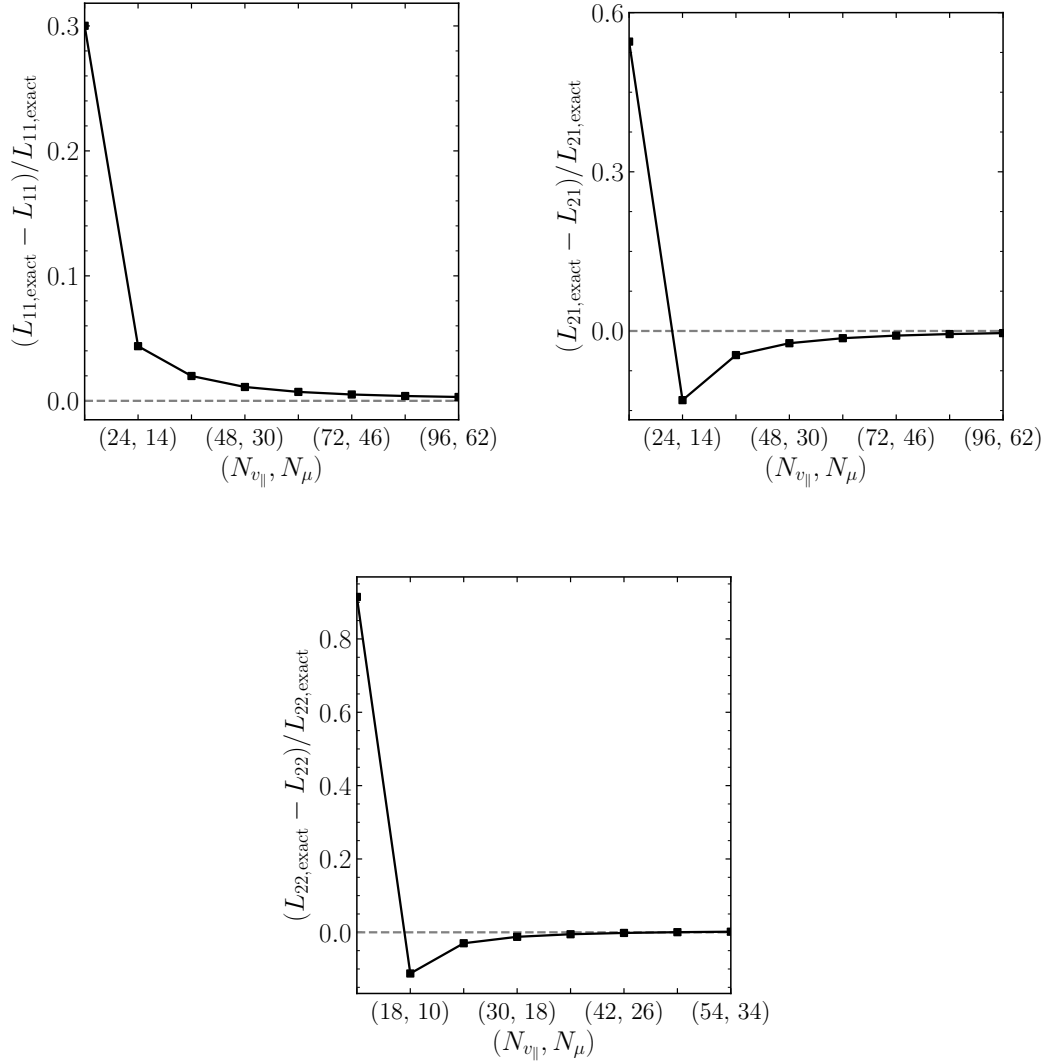


Figure 9.8: Velocity space resolution scans of errors in the Spitzer transport coefficients for the collision model with terms up to the $\{j = 2, l = 1\}$ term in the field particle operator, relative to coefficients determined with the exact Fokker-Planck operator by Belli and Candy (2011). *Top left:* scan for L_{11} . *Top right:* $L_{12} = L_{21}$. *Bottom:* L_{22} .

Parameters of linear Cyclone Base Case simulations

Cyclone Base Case:

$\tilde{r} = r/a$	0.5
$\tilde{R} = R_0/a$	2.77778
$d\tilde{R}/d\tilde{r}$	0
q	1.4
$\hat{s} = d \ln q / d \ln r$	0.8
κ	1.0
n_i/n_e	1
T_i/T_e	1
m_i/m_e	3672
$-d \ln T_i / d\tilde{r}$	2.49
$-d \ln T_e / d\tilde{r}$	2.49
$-d \ln n_i / d\tilde{r}$	0.8
$-d \ln n_e / d\tilde{r}$	0.8

Common run parameters:

$\nu_{ii}a/v_{th,r}$	0.1
$\Delta t v_{th,r}/a$	0.008
$v_{c,\perp}/v_{th,s}$	3.0
$v_{c,\parallel}/v_{th,s}$	3.0
$N_{\text{period}} \times N_z$	3×24

stella run parameters:

μ -grid	Gauss-Quad.
$N_{v_{\parallel}}$	48
N_{μ}	12

GS2 run parameters:

N_{gauss}	20
N_E	32

Table 9.1: Parameters of linear Cyclone Base Case simulations with **stella** and **GS2**. The quantities r and R are the minor and major radius of the chosen flux surface of the DIII-D tokamak, respectively, q denotes the safety factor, $\hat{s}$ is the magnetic shear, κ is the flux surface elongation, a is the reference length, chosen to be the minor radius of the last-closed-flux-surface and $v_{th,r}$ is the reference speed, chosen as $v_{th,r} = \sqrt{2T_{\text{ref}}/m_{\text{ref}}}$ with $T_{\text{ref}} = T_i$ and $m_{\text{ref}} = m_i$.

CHAPTER 10

CONCLUSION

We have developed a collision model for the gyrokinetic solver `stella` that satisfies pertinent conservation laws and Boltzmann’s H-theorem and provides a rigorous approximation of the linearised Fokker-Planck operator. Multiple plasma species are supported by the collision model, with full intra- and inter-species collisions taken into account, irrespective of the species mass ratios. In line with `stella`’s mixed implicit-explicit numerical scheme, the collision model makes use of an implicit algorithm to avoid a CFL constraint on the maximum timestep size. The diffusive, test-particle component of the linearised Fokker-Planck operator, which describes the diffusion of energy and scattering of pitch angles due to collisions, is treated exactly. The field-particle piece of the operator is approximated using series expansions in spherical harmonics and the Hirshman-Sigmar basis functions that are precomputed recursively from error functions during code initialisation. The expansion of the field-particle operator thus obtained reduces the integrodifferential exact field-particle operator to an integral operator that is amenable to implementation in an implicit scheme. A Green’s function method was employed for this purpose. To the best of the author’s knowledge, the collision model described here constitutes the first implementation in a gyrokinetic code of a model collision operator with scalable accuracy that rigorously approximates

the Fokker-Planck operator. In the limit where only the first two terms in the series expansion are retained, the collision model reduces to the energy- and momentum-conserving model commonly employed in gyrokinetic codes (cf. Abel et al., 2008; Barnes et al., 2009; Sugama et al., 2009). Benchmarks against the collision model of the gyrokinetic code **GS2** for both ion- and electron scale turbulence confirm that this is the case. The classical Spitzer problem was solved to demonstrate the scalable accuracy of the collision operator employed here; including the collisional energy-flux and higher-order terms in the field particle operator yields residuals in the Spitzer coefficients below 1%, measured with respect to Spitzer coefficients obtained with the exact Fokker-Planck operator by Belli and Candy (2011).

Several improvements can be made to the collision model to increase numerical performance and physical fidelity: the self-adjointness of the collision operator implies that the discretisation matrix, R , of the test-particle component is symmetric, as described in Section 8.1. For the numerical scheme employed on uniform velocity grids, the symmetry $R = R^T$ is exact; on non-uniform grids, where $R \approx R^T$, symmetry could be enforced via $R \rightarrow R' := \frac{1}{2}(R + R^T)$. At present, an LU-decomposition of R is employed to solve the implicit Euler equations during the collisional time advance. The symmetry of R can, however, be exploited by using a Cholesky decomposition of R , provided that R is positive-definite. Determining if or under what conditions this is the case is worth investigating since the Cholesky algorithm reduces the solve complexity and memory usage by a factor of two compared to the LU algorithm. The exact symmetry of R also permits the use of the Cuthill-McKee bandwidth-reducing algorithm (Cuthill and McKee, 1969). The upper and lower bandwidth of R is given by $w = N_\mu + 1$, with nine non-zero bands for the three-point stencils employed in the discretisations. Since the band-matrix LU-solve complexity scales with wN_μ , a bandwidth reduction may provide significant performance

gains for large N_μ . At the time of this writing, **stella** solves the gyrokinetic equation in the electrostatic limit. Development is currently in progress to include electromagnetic effects (no involvement of the author). This requires that the collision model introduced here is compatible with the electromagnetic algorithm; a modification of the time advance equations to account for the vector potential may be required. Finally, the collision model introduced here would benefit from an extension to the case of unequal species temperatures since $T_e = T_i$ does not always hold in a reactor, in particular in reactor edge regions. If $T_e \neq T_i$, the test-particle and field particle operators, and the self-adjointness relations of the field-particle operator, are modified (cf. Abel et al., 2008; Sugama et al., 2009).

Recent work with an exact, explicit implementation of the Fokker-Planck operator in the **GENE** code (Pan et al., 2020) has demonstrated that an exact treatment of the field-particle operator can yield significant corrections to TEM instabilities and zonal flow damping in tokamaks (Pan et al., 2021), compared to an energy and momentum conserving collision model. It may be useful to benchmark the collision model introduced here against these findings to verify how many terms in the field-particle operator are required to achieve the fidelity of the exact operator in realistic simulations of turbulence. Upcoming work by the author with collisional **stella** may focus on gyrokinetic simulations of the transport of impurity ion species in W7-X. Impurities such as Carbon, Argon, Iron, or Tungsten can have a high collisionality due to their high ion charge. The transport of such impurity species must be controlled in magnetic confinement reactors to avoid impurity accumulation in the plasma core, where highly charged species lead to a rapid radiative energy loss of the plasma. Measurements of the diffusion coefficients of iron ions, injected by laser ablation in W7-X, exceed neoclassical predictions by two orders of magnitude (Langenberg et al., 2018; Geiger et al., 2019). This suggests that

turbulence plays an important role in the transport of impurities. Indeed, gyrokinetic simulations of impurity transport in W7-X performed with **stella** (García-Regaña et al., 2020) indicate that turbulence can explain the measured levels of transport. These simulations have, however, been collisionless, motivating a collisional gyrokinetic investigation. This would also test the theoretical prediction, based on a quasi-linear calculation, that the effect of collisions on the impurity flux is relatively small (Buller and Helander, 2020) at reactor-relevant conditions. Finally, the implementation of an accurate collision model is a significant step towards the inclusion of neoclassical effects in the thus far purely gyrokinetic code **stella**.

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