Dust-Plasma Interactions In The Plasma Edge Region

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Abstract

*I will show you fear in a handful of dust*

T.S. Elliot

This thesis concerns the interaction of small, particulate, solid matter - ‘dust’ - with plasmas, in the plasma edge region where such dust is commonly found. Dust in this region can have a significant impact on a variety of industrial plasma applications, and it is low-temperature industrial plasmas that form the focus of this work.

A novel model for the sheath region at the edge of a plasma is proposed, to account for the loss of electrons at the plasma boundary. This is then compared to an existing Boltzmann electron model; significant differences are noted in the sheath structure, and consequently the charging and dynamics of dust in the plasma sheath.

The effect of sparse ion collisions in the vicinity of a dust grain near the plasma edge is also investigated. The strong plasma flow in the edge region is found to significantly increase collisional charging of dust grains. Somewhat counter-intuitively, it is found that even sparse collisions can play a significant (and in fact dominant) role in the charging and shielding of dust grains at the edge of a plasma. The length-scale over which the charge on such grains is shielded by the plasma is found to be significantly less than the Debye length. Together, the altered grain charging and shielding behaviour have the potential to fundamentally alter how dust grains interact with edge-plasmas.
Acknowledgements

There are quite a number of people whom I would like to take this opportunity to thank for their help and support during my PhD.

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</tr>
<tr>
<td>$\lambda_{De}$</td>
<td>Electron Debye length (evaluated at sheath edge)</td>
</tr>
<tr>
<td>$\lambda_i$</td>
<td>Spatial scale of presheath</td>
</tr>
<tr>
<td>$\lambda_{mfp}$</td>
<td>Ion mean free path</td>
</tr>
<tr>
<td>$T_e$</td>
<td>Electron temperature</td>
</tr>
<tr>
<td>$T_i$</td>
<td>Ion temperature</td>
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<tr>
<td>$T_n$</td>
<td>Neutral gas temperature</td>
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<tr>
<td>$n_o$</td>
<td>Electron (or ion) number density at sheath edge</td>
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<td>$n_i$</td>
<td>Ion number density</td>
</tr>
<tr>
<td>$n_e$</td>
<td>Electron number density</td>
</tr>
<tr>
<td>$e$</td>
<td>Magnitude of electron charge</td>
</tr>
<tr>
<td>$\epsilon_o$</td>
<td>Permittivity of free space</td>
</tr>
<tr>
<td>$k_B$</td>
<td>Boltzmann’s constant</td>
</tr>
<tr>
<td>$\Phi_p$</td>
<td>Potential of core plasma (relative to sheath edge)</td>
</tr>
<tr>
<td>$r_d$</td>
<td>Dust grain radius</td>
</tr>
<tr>
<td>$n_e \text{ peak}$</td>
<td>Peak electron density over RF oscillation</td>
</tr>
<tr>
<td>$\nu_{coll}$</td>
<td>Charge-exchange collision frequency</td>
</tr>
<tr>
<td>$\omega_{pe}$</td>
<td>Electron plasma frequency</td>
</tr>
<tr>
<td>$\omega_{pi}$</td>
<td>Ion plasma frequency</td>
</tr>
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<td>$\omega_{rf}$</td>
<td>RF oscillation angular frequency</td>
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<td>$m_i$</td>
<td>Ion mass</td>
</tr>
<tr>
<td>$V_{rf}$</td>
<td>RF driving voltage applied to wall</td>
</tr>
<tr>
<td>$v_B$</td>
<td>Bohm speed</td>
</tr>
<tr>
<td>$v_i$</td>
<td>Ion speed</td>
</tr>
<tr>
<td>$\Phi_{dc}$</td>
<td>Time averaged sheath potential</td>
</tr>
<tr>
<td>$x$</td>
<td>Distance from sheath wall</td>
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</table>
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<table>
<thead>
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<th>Symbol</th>
<th>Description</th>
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<tr>
<td>$f$</td>
<td>Velocity distribution function</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Normalising constant (see §2.1.3)</td>
</tr>
<tr>
<td>$v_{ex}$</td>
<td>Electron speed in the x-direction</td>
</tr>
<tr>
<td>$v_{eo}$</td>
<td>Electron speed (in x-direction) at sheath edge</td>
</tr>
<tr>
<td>$m_e$</td>
<td>Electron mass</td>
</tr>
<tr>
<td>$V_{dc}$</td>
<td>Time averaged potential on wall (relative to sheath edge)</td>
</tr>
<tr>
<td>$V_{wall}$</td>
<td>Instantaneous potential on wall</td>
</tr>
<tr>
<td>$t$</td>
<td>Time</td>
</tr>
<tr>
<td>$J_i$</td>
<td>Ion current density to wall</td>
</tr>
<tr>
<td>$J_e$</td>
<td>Electron current density to wall</td>
</tr>
<tr>
<td>$v_{te}$</td>
<td>Electron thermal speed</td>
</tr>
<tr>
<td>$v_o$</td>
<td>Speed of particle entering dust grain potential well</td>
</tr>
<tr>
<td>$v_g$</td>
<td>Speed of particle at dust grain surface</td>
</tr>
<tr>
<td>$\phi_d$</td>
<td>Potential of dust grain (relative to local plasma)</td>
</tr>
<tr>
<td>$q_j$</td>
<td>Charge of species $j$ (ion or electron)</td>
</tr>
<tr>
<td>$b_{crit}$</td>
<td>Critical impact parameter for collision</td>
</tr>
<tr>
<td>$\sigma_j$</td>
<td>Dust grain collision cross-section for species $j$</td>
</tr>
<tr>
<td>$I_j$</td>
<td>Current to dust grain from species $j$</td>
</tr>
<tr>
<td>$Q_d$</td>
<td>Charge on dust grain</td>
</tr>
<tr>
<td>$E_s$</td>
<td>Typical sheath electrostatic field</td>
</tr>
<tr>
<td>$W_s$</td>
<td>Work done by sheath field</td>
</tr>
<tr>
<td>$W_d$</td>
<td>Work done by dust grain</td>
</tr>
<tr>
<td>$L$</td>
<td>Angular momentum</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Torque</td>
</tr>
<tr>
<td>$v_r$</td>
<td>Speed in radial direction (relative to dust grain)</td>
</tr>
<tr>
<td>$E_r$</td>
<td>Radial electrostatic field surrounding a dust grain</td>
</tr>
<tr>
<td>$F$</td>
<td>Force on a particle/dust grain</td>
</tr>
<tr>
<td>$F_e$</td>
<td>Electrostatic force</td>
</tr>
<tr>
<td>$F_g$</td>
<td>Gravitational force</td>
</tr>
<tr>
<td>$F_{id}$</td>
<td>Ion drag force</td>
</tr>
</tbody>
</table>
List of Symbols

$E_{\text{neut}}$  
Neutral drag force

$t_i$  
Quantised time points in RF oscillation

$\alpha'$  
Normalising factor (see §3.1)

$F_o'$  
Normalising factor (see §3.1)

$v_{\text{cut}}'$  
Electron cutoff speed

$\alpha$  
Altered normalising factor (see §3.2)

$F_o$  
Altered normalising factor (see §3.2)

$v_{\text{cut}}$  
Altered electron cutoff speed (see §3.2)

$\Phi_{\text{min}}$  
Minimum instantaneous sheath potential

$I_o$  
Collection of constants (see §3.3)

$v_{\text{min}}$  
Minimum electron speed to collide with dust grain

$\phi_{d\text{ CC}}$  
Dust grain potential (Cutoff electron model)

$\phi_{d\text{ BE}}$  
Dust grain potential (Boltzmann electron model)

$v_{\text{dust}}$  
Dust grain speed

$E_{\text{tot}}$  
Total ion energy (kinetic & potential)

$r$  
Distance from dust grain

$\theta$  
Angle about dust grain (relative to ion flow)

$Q_t$  
Trapped ion charge within region

$Q_u$  
Untrapped ion charge within region

$Q_e$  
Electron charge within region

$\sigma_{\text{trap}}$  
Cross-section for trapped ion collection

$\sigma_{\text{max}}$  
OML cross-section for Maxwellian ions

$\nabla P$  
Pressure gradient

$E$  
Electrostatic field

$r_o$  
Ion initial radial position

$\theta_o$  
Ion initial azimuthal position

$N_i$  
Number of ions

$b$  
Impact parameter

$db$  
Increment between adjacent ion impact parameters

$l$  
Index of radial point $r_l$
**List of Symbols**

$m$ \quad \text{Index of azimuthal point } \theta_m

$\delta t_{l,m}$ \quad \text{Time increment spent in grid point } l,m

$N_r$ \quad \text{Number of radial gridpoints}

$N_\theta$ \quad \text{Number of azimuthal gridpoints}

**Abbreviations**

OML \quad \text{Orbital Motion Limited}

ABR \quad \text{Allen, Boyd, and Reynolds}

OM \quad \text{Orbital Motion}

BE \quad \text{Boltzmann Electron (model)}

CC \quad \text{Cutoff-Corrected (model)}

RF \quad \text{Radio Frequency}

**Normalisations**

Speed: $\tilde{v} = \frac{v}{v_{te}}$

Density: $\tilde{n} = \frac{n}{n_o}$

Electrostatic potential: $\tilde{\phi} = \phi \frac{e}{k_B T_e}$

Distance/length: $\tilde{x} = \frac{x}{\lambda_{De}}$

Time: $\tilde{t} = \frac{t v_{te}}{\lambda_{De}}$

Force: $\tilde{F} = F \frac{\lambda_{De}}{k_B T_e}$

Current density: $\tilde{J} = \frac{J}{en_o v_{te}}$
Chapter 1

Introduction

Plasma is a state of matter consisting of partially or fully ionised gas. While plasmas have no overall charge, they are made up of constituent populations of positively and negatively charged particles, typically ions and electrons, which interact via the electromagnetic force and respond collectively to any applied electric or magnetic fields. As a result, plasmas exhibit a greater and more complex array of phenomena than ordinary gases.

Plasmas exist across a wide range of conditions, as any gas with the energy to ionise sufficiently may form a plasma. As a result, plasma is the most abundant form of (baryonic) matter in the Universe [6].

1.1 Terrestrial Plasmas

While naturally occurring plasmas are common in space, they are far less so on Earth. However, plasmas are created artificially for a wide variety of industrial purposes.

Plasmas are most notably used in industry for semiconductor manufacturing, which is achieved through plasma etching and deposition techniques [7]. These techniques, and others, are also used in plasma surface modification of biomaterials, allowing the surface properties of implants and prostheses to be altered without altering the internal properties of the materials [8], as well as in the aerospace and automotive industries [1].

Other industrial plasma applications include the manufacture of ozone for decontamination of drinking water [9], creation of stronger plastics via plasma polymerisation, sterilisation of medical equipment, and numerous others [7, 10].
In addition, various forms of fusion reactors exist to create energy via the confinement of a high temperature deuterium-tritium plasma [11]. At sufficiently high temperatures, deuterium and tritium undergo nuclear fusion, joining to create helium and releasing an energetic neutron particle in the process:

$$^2_1D + ^3_1T \rightarrow ^4_2He + ^1_0n + 17.6 \text{ MeV}. \quad (1.1)$$

Attempts to exploit this process as an energy source have been ongoing for some time. Of the various current approaches to achieving fusion, magnetic confinement techniques are most relevant to this work. This approach is most commonly used in doughnut-shaped tokamak or stellarator reactors, and involves the use of a strong magnetic field to confine the hot plasma away from the reactor wall.

1.2 Plasma Boundary

Apart from some transient plasmas created by inertial confinement techniques, most plasmas typically have to be bounded by a solid wall to confine the plasma from the outside environment. The edge of a plasma bounded by a solid wall presents a far more complex region than is the case with a neutral gas.

Solid surfaces act as sinks for incoming charged particles; electrons are typically absorbed by the wall, while ions may be absorbed by the wall (depending on the ion species and wall material) or neutralised without absorption to become a gaseous atom. In either case, the incident particle is lost to the plasma, while its charge is transferred to the wall.

Unless the ion temperature far exceeds the electron temperature in a plasma, electrons are typically the faster moving species. As such, the electron flux to a wall will exceed the ion flux and the surface draws a net negative current from the plasma. As the surface becomes negatively charged, it repels incoming electrons and attracts ions, reducing the electron current it draws and increasing the ion current until it reaches current-balance [12].

1.2.1 Sheath and Presheath

A ‘sheath’ region forms at the interface between a plasma and any solid surface. The negative charge on the wall causes a region of positive space-charge to form in front of
it as electrons are repelled from the surface, while ions are attracted towards it [13]. This positively charged region acts to ‘shield’ the plasma from the negative charge on the wall. This is one of the key behaviours distinguishing a plasma from a regular gas - the ability to move collectively to screen out electric fields within the plasma.

In the simplest example, we can derive this shielding behaviour following the approach of Chen [14]. We only consider shielding due to electrons, since they are the more mobile species, while ions are assumed to be immobile over the timescales in which the electrons move to shield the wall charge. The resulting Debye-Hückel potential (derived in full in appendix A) is an approximate solution for the potential profile adjacent to a charged surface:

$$\Phi(x) = V_{\text{wall}} \exp \left( \frac{-x}{\lambda_{\text{De}}} \right)$$

(1.2)

where $x$ is distance from the wall and $V_{\text{wall}}$ is the potential at the wall (relative to a reference potential $\Phi = 0$ far away). Since ions are not truly immobile and are attracted to the wall, this model is limited in validity. However, it does give the spatial scale over which charges are typically shielded in a plasma, the Debye length - a crucial length scale throughout this work:

$$\lambda_{\text{De}} = \sqrt{\frac{\epsilon_o k_B T_e}{n_0 e^2}}$$

(1.3)

where $\epsilon_o$ is the permittivity of free space, $k_B$ is Boltzmann’s constant, $T_e$ is the electron temperature, $n_0$ is the electron density at the sheath edge, and $e$ is the magnitude of the electronic charge.

In the real sheath, the wall’s role as a sink for incident ions causes a further boundary region to exist, beyond the sheath’s space-charge region. This ‘presheath’ region is quasi-neutral (i.e. contains approximately equal ion and electron charge densities) and typically far wider than the sheath [15, 16]. The spatial scale of the presheath, $\lambda_i$, is typically the mean free path for either ion-neutral collisions or electron-neutral ionisation, depending on which type of collision is dominant in the plasma. A weak electric field exists in the presheath region, which accelerates incoming ions towards the wall in order for the ion current to equal the electron current to the wall. These features are shown qualitatively in figure 1.1.

Since the presheath is typically so much larger than the sheath region, they are often considered separately in a ‘two-scale’ approach [15]. The two-scale approach assumes
the asymptotic limit of $\lambda_D/\lambda_i \to 0$, in which case the sheath appears (on the presheath scale) as an infinitely thin region adjacent to the wall where the electric field reaches a singularity. On the sheath scale, the potential decays asymptotically towards $\Phi = 0$, and the sheath edge on this scale is infinitely far away. The plasma region where $n_i \neq n_e$ is, in this limit, confined to the sheath.

Figure 1.1: Diagram of plasma boundary, showing the sheath and presheath regions; adapted from Lieberman and Lichtenberg (2005) [1]. Ion and electron densities ($n_i$ and $n_e$ respectively) are shown in the top graph, while the decaying potential $\Phi$ surrounding the wall is shown in the bottom graph (relative to the sheath edge where $\Phi = 0$).

In a real plasma boundary, the sheath smoothly transitions into presheath and the abrupt distinction made between the two regions is somewhat artificial; there is always some residual charge imbalance within the presheath, and the exact transition point between the two regions cannot easily be distinguished.

The Bohm criterion - equation 2.3 - which states that ions cross the sound speed at the exact point that quasineutrality breaks down (i.e. the sheath edge) is another
consequence of the abrupt separation of these regions in the two-scale limit (or, more formally, the condition that \( \partial \tilde{\Phi} / \partial \tilde{x} = 0 \) at the same position that \( \tilde{\Phi} = 0 \), as used in the derivation in Appendix A).

However, since \( \lambda_{De} \ll \lambda_i \) much of the time, it is convenient and generally accurate to discuss these two regions separately, and the larger the difference between the two scale-lengths \( \lambda_{De} \) and \( \lambda_i \), the more distinct the division between sheath and presheath.

As the plasma will typically be in contact with the wall over a scale \( L \gg \lambda_{De} \), corners and other geometric effects can often be ignored, and the wall modelled as an infinite planar surface. As a result, the sheath can typically be considered in one-dimension, with variation in the plasma occurring in only the \( x \)-direction (the direction perpendicular to the wall, as shown in figure 1.1).

This sheath region may be further complicated by a range of additional processes [17, 1], such as re-ionisation of neutral atoms near the wall, the emission of secondary electrons from the wall due to the impact of energetic plasma particles, thermionic emission of electrons from a hot wall, or the imposition of a time-varying voltage on the wall (as is common in industrial discharges).

The sheath region is of interest for numerous plasma applications, as one may form whenever a solid surface is brought into contact with a plasma. Sheath processes are particularly important in the industrial plasmas used for semiconductor etching and other surface modification applications, as the plasma-surface interaction is the main focus of the application. In the case of semiconductor etching, it is the acceleration of ions in the sheath’s electrostatic field which allows the highly accurate etching of surfaces required to make increasingly small features in electronic devices [7].

However, the sheath is also of more general interest interest for modelling the edge of a magnetically confined fusion plasma and its interaction with the reactor wall, or for determining the charging of objects such as comets or man-made satellites in astrophysical plasmas.

### 1.2.2 Radio-Frequency driven plasma sheath

A laboratory plasma may be created by the application of a constant (DC) voltage across the gas [18]. In this case, one (or both) walls of the plasma are actively biased by application of a current to the wall. Rather than reaching the steady-state ‘floating’
potential relative to the plasma, at which the wall draws no net current from the plasma (as described above), such a wall can have its potential externally set by changing the external power applied to the wall.

In industrial applications, many plasmas are driven by the application of an oscillating, radio-frequency (RF) potential to one wall, rather than a DC voltage [19], and 'capacitively coupled' RF-driven sheaths will form a core part of this work. In such a plasma, the amplitude of the wall potential oscillates at the RF frequency and, consequently, so does the position of the sheath edge. Since the sheath potential acts to reflect incoming electrons back into the plasma, electrons reflected off this oscillating front can undergo collisionless heating [20], contributing to a higher ionisation efficiency and (along with other effects) allowing RF discharges to operate at lower pressures than DC-driven ones [19].

A matching network and a coupling capacitor in the system prevent any conduction current flowing in the circuit; thus, the wall still reaches a (modified) floating potential, and draws no net current from the plasma [18]. This is discussed in more detail in Chapter 2.

RF-driven plasmas may also be 'inductively-coupled', rather than capacitively, in which case the plasma is driven by absorption of RF waves from an antenna through which an oscillating current is passed [20], however such plasmas are not of direct relevance to this work. Other complicating effects such as magnetisation of the edge plasma (which produces an additional transition layer between the sheath and presheath) can also arise in certain settings, but are not discussed here.

A table of typical parameters for dust plasma experiments from several experimental papers (carried out in capacitively-coupled Argon or Argon-Silane plasmas) are detailed in the table below. Parameters from within this range are used in the later Chapters for simulations:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Typical Value Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Background neutral density</td>
<td>0.1 - 20 Pa [21, 22, 23]</td>
</tr>
<tr>
<td>Electron number density</td>
<td>0.2 - 12 x 10^{15} m^{-3} [22, 24, 23]</td>
</tr>
<tr>
<td>Electron temperature</td>
<td>2 - 10 eV [25, 22, 23]</td>
</tr>
<tr>
<td>RF amplitude</td>
<td>20 - 250 V [21, 24, 23]</td>
</tr>
<tr>
<td>RF frequency</td>
<td>13.56 MHz [25, 22, 23]</td>
</tr>
</tbody>
</table>
1.3 Dust in Plasmas

Dust is ubiquitous in plasmas, with almost all plasmas containing some degree of dust. It is a common feature in space plasmas, including in interstellar clouds [26], the collapse of which is key to the formation of stellar systems. Interplanetary dust also exists throughout our own solar system. For instance, dust is produced by the erosion of comets near the sun, and the rings of the gas giant planets are also comprised of small, solid particles [27]. The radial spokes visible in the rings of Saturn (figure 1.2) are a notable example of a dust-plasma phenomenon which is explained via the electromagnetic interactions of charged dust particles in Saturn’s magnetosphere [28, 26].

Terrestrial plasmas are also often contaminated by small solid impurities [29], despite stringent measures to ensure a clean environment in industrial and fusion plasmas. This is because plasmas can produce dust either from sputtering and erosion of surfaces in contact with the plasma [30, 31], or aggregation of dust inside the plasma [24, 6]. Since these processes allow almost any plasma to act as a source of its own dust, it is very difficult indeed to achieve a completely dust-free plasma.
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Figure 1.3: Dust levitating in the sheath field just above the lower electrode of a low-temperature plasma discharge. Reproduced from Ticos (2013) [3].
In this example, the dust was intentionally added to the plasma. As can be seen, the dust has also arranged itself into a regular lattice, known as a ‘dust crystal’.

In manufacturing plasmas, such as thin-film deposition and semiconductor processing plasmas, dust is typically trapped in the sheath region and may fall onto the surface being processed, causing contamination and loss of the product [32]. This problem has been brought under control in the industry, by altering the geometry of the sheath field to localise the trapping of dust particles [33] and suppressing the growth of dust in the plasma [6]. However, it is still an important and costly issue in the industry [34, 35], and one that has the potential to grow as increasingly small pathway sizes on silicon chips cause smaller-scale dust grains to become a problem [33].

An example of dust-trapping in the plasma sheath can be seen in figure 1.3, which shows dust levitating above the lower electrode of an industrial plasma.

In tokamak plasmas, dust can also be of importance [36]. Contamination of the core plasma with high atomic-number elements can significantly increasing radiative cooling, and at sufficient concentrations may even terminate the plasma. Dust-induced plasma termination has been seen in the LHD stellarator, where the termination of certain long-pulse discharges was observed to occur due to the entrance of iron dust into the core plasma [37].

In the case of tungsten, one of the planned wall materials for the ITER tokamak, the core plasma will not tolerate a tungsten concentration above 1 part in $10^5$ (by number) [38]. In the plasma to be produced by ITER, this corresponds to approximately 0.6μg of tungsten, equivalent to a single dust grain of radius 0.2mm entering the core plasma.
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[39]. Beryllium is another of the planned wall materials for ITER, with the advantage of a much lower atomic number, but the disadvantage that beryllium dust is highly toxic [40].

In addition, dust in the tokamak may also absorb radioactive tritium from the plasma, depleting the tokamak of fuel while increasing the tritium content of the reactor above intended levels [31].

The presence of dust can, however, also be advantageous. Controlled introduction of dust into the manufacturing of nanostructured silicon (used in solar cells) can increase the rate of crystallisation [41], and lower the number of defects in the crystal [32]. Dust has also been used as a sheath diagnostic since, by tracking the motion of dust in the sheath field, the shape and spatial extent of the sheath can be determined [23]. Dust has even been manufactured intentionally in plasmas, with various surface coatings applied to modify its properties as desired. For example, a deposition of a catalytic coating on the surface allows the dust to act as a high surface-area catalyst for chemical reactions [42, 43]. The discovery of dust-plasma crystals, regular lattices of dust particles analogous to atomic crystal structures (such as shown in figure 1.3), also allow various thermodynamic and hydrodynamic processes to be investigated at the single-particle level due to their much larger scale than conventional crystal structures [44].

To do any of this, however, the interaction between the dust and the sheath must be accurately understood, particularly the charge acquired by the dust from the absorption of plasma particles in the sheath.

1.3.1 Dust Charging

Dust in a plasma becomes charged by absorption of plasma particles, in a similar manner to the wall at the plasma boundary. The charge acquired by the dust is a key factor in determining its interactions with the plasma, particularly its dynamics within the plasma, and thus where dust contamination is likely to be greatest.

Several theories exist for modelling the charging of dust in a plasma. The Orbital Motion Limited (OML) theory was developed by Mott-Smith and Langmuir in 1926 [45]. It is a relatively simple theory, making no attempt to calculate the potential distribution surrounding the grain. OML calculates a collision cross-section for plasma particles approaching the charged grain, based solely on conservation of energy and angular momentum. From these cross-sections, and the ion and electron velocity distributions,
it can then calculate the respective currents from each plasma species to the grain [46].

OML is the most widely used charging theory, due in part to its simplicity and the ease with which it can be adapted to different situations. As such, it is also the charging theory used and compared to throughout this work. The OML theory is most applicable for small dust grains of radius $r_d \ll \lambda_{De}$ and non-flowing plasmas, however variants also exist for dust $r_d \gg \lambda_{De}$ and flowing plasmas [47], and it can relatively easily be adapted to different velocity distributions (as seen in Chapter 3). However, since OML does not attempt to calculate the potential distribution around the grain, it cannot predict the existence of so-called absorption radii [48], which effectively increase the collision-cross section for ions (or electrons if the grain is positively charged) if the potential around the charged grain varies more steeply than $1/r^2$. These are discussed in more detail in Section 2.3.2, along with other limitations to the OML approach.

The Allen, Boyd, and Reynolds (ABR) theory is an alternative dust charging theory for plasmas with cold ions [49]. In the ABR model, ions are attracted directly towards the charged dust grain and move only radially, while electrons are considered to be in thermal equilibrium and described by a Boltzmann distribution. This theory can predict the shape of the sheath and presheath surrounding the grain, as well as the charge acquired by the grain. However, its radial motion approach, and hence disregard for ion angular momentum, limit its usefulness.

While a cold ion model will be used later in this work to model the plasma edge, the radial motion approach is inappropriate for dust in this region due to the strong ion flows present in the sheath.

The full Orbital Motion (OM) theory is the final, and most complicated, charging theory we will discuss. This approach involves a complete, self-consistent solution to the collisionless Vlasov-Poisson equation for ions in the dust grain potential well [48].

This approach still assumes spherical symmetry and conservation of angular momentum, neither of which are true in the sheath. Due to this, and its vastly increased complexity, this approach is not taken in favour of the simpler OML theory, which is derived in detail in Chapter 2.
1.4 Focus of this work

This work focuses on the charging of small (sub-Debye length) dust grains in the plasma sheath region. Most previous work on dust has been done in the bulk plasma away from the sheath, however it is also crucial to consider dust at the plasma edge.

Two different topics are studied in detail, both relating to the dust-plasma interaction in the plasma sheath. The first of these is the assumption of electron thermal equilibrium within the sheath. A set of parameters are identified for which this assumption breaks down and incorrectly predicts both the sheath structure and the charging of dust grains in the sheath. This in turn has consequences for the dynamics of charged dust grains in this region.

Secondly, the effect of ion-neutral collisions on dust grain charging is investigated. Collisional effects are often ignored by standard dust charging theories such as ABR, OML, and even the complete OM charging theory. However, previous work in the non-flowing bulk plasma has shown that ion-neutral collisions may be important even in low-collisionality plasmas. This is investigated in the strongly flowing edge plasma, where it is found to significantly affect the dust-plasma interaction.

1.4.1 Modelling of the Sheath

Many sheath models treat electrons as being in thermal equilibrium [50, 51, 25, 52], based on two main assumptions: first that the low inertia of the electrons allows them to reach an equilibrium much faster than any other relevant sheath timescales, and second that a negligibly small fraction of electrons entering the sheath region are absorbed by the solid wall.

Sometimes even simpler models are used, such as the Child-Langmuir model [53] which entirely neglects the electron contribution when solving Poisson’s equation for the sheath profile, or the parabolic approximation presented by Tomme et al.[32] which shows that many sheath models can be approximated with good accuracy by appropriately fitted parabolas. However, even the more rigorous analytic approximations derived by Riemann [54], which consider various types of sheath and include effects such as ionisation and collisions, assume thermal equilibrium and use Boltzmann distributed electrons.

Often the thermal equilibrium model is sufficient as the much greater mobility of electrons than ions means that:
1) They respond very rapidly to any changes in the sheath field, which they experience as a quasi-static conservative field.

2) They cause the wall to charge up negatively, so that few electrons have sufficient energy to surmount the sheath potential barrier and reach the wall; This renders electron absorption by the wall negligible (compared to the rate at which electrons enter the sheath from the plasma-side).

However, many industrial and laboratory plasmas are driven by oscillating radio-frequency (RF) potentials applied to the wall of the plasma container. When large RF driving potentials are applied, the resulting nonlinear electron fluid oscillations cause the assumption of negligible wall-absorption to break down, rendering the Boltzmann model invalid. It is the sheath formed adjacent to such a wall which will be considered in this work.

Applying an oscillating RF voltage to the wall causes the average potential on the wall, $V_{dc}$, to become more negative, as will be seen in section 2.2. This would seem to increase the potential barrier experienced by electrons, and ensure that only a negligible fraction reach the wall. However, this increase in $V_{dc}$ is smaller than the imposed RF voltage, $V_{rf}$. Consequently, for higher RF voltages, the amplitude of the potential oscillation on the wall can become (almost) as great as the negative DC wall potential ($V_{rf} \approx V_{dc}$) [55].

Thus, near the peak of an RF cycle, the potential barrier experienced by the electrons briefly becomes small, causing a large increase in electron density deep in the sheath and allowing many more electrons to reach the wall during this time [56]. Since the electron flux to the wall (and also to any dust grains in the sheath) is very low throughout the rest of the RF cycle, this period - despite its brevity - has a significant effect on both wall and grain charging.

At sufficiently high RF voltages, the electron density, $n_e$, at the peak of the RF oscillation can become high enough to exceed the ion density, $n_i$, near the wall (unlike most of the cycle, where electrons are repelled from the wall and $n_e \ll n_i$). This brief peak in electron density can result in the formation of a transient double charge layer in the sheath around the peak of the RF oscillation. Away from the wall, the ion density remains greater than the electron density. However, close to the wall where the ion density is low, it is exceed by the electron density.

This double charge layer causes an electric field reversal within the sheath. The sheath potential profile therefore does not decrease monotonically from the plasma to the wall, but has a lower minimum within the sheath. This is discussed in detail in
CHAPTER 1. INTRODUCTION

section 3.3, and depicted in figure 3.6.

This effect increases the potential barrier experienced by the electrons and reduces electron current to the wall. The excess ion current to the wall then causes the wall to charge more positively than would otherwise be expected. Another result of this field-reversal is that the electrons that do pass the potential minimum are no longer repelled from the wall, but instead attracted towards it, much like the ions. Therefore, the assumption of thermal equilibrium for electrons become completely invalid in this situation.

Valentini et al.[57] attempted to account for this effect via a model where the electrons received a Boltzmann treatment between the sheath edge and the potential minimum, and had the same freefall model as the ions applied from the minimum to the wall. This is significantly better for providing spatial potential profiles than the Boltzmann approximation, and demonstrates both the field reversal and the altered wall charging that results from it. However, this approach overestimates the electron density at the field reversal point by up to a factor of two, while also overestimating the rate at which electron density falls off within the field-reversed region. The work also does not address the effect the altered electron population has on dust grain charging in the sheath.

The field-reversal scenario is also quite beyond the remit of many of the simpler approximations used, such as Tomme et al.’s parabolic fits. Kinetic simulations are quite capable of accurately including this physics (and much more), however they cannot distinguish between the effect of electron loss to the wall and the variety of other physics included. These simulations are also far more complicated and computationally expensive to carry out. The approach used in this work allows a direct investigation of the consequences when the assumption of no wall-absorption is dropped, and provides a relatively simple model to treat the electron distribution in this instance.

As the overall fraction of the electron population which is lost to the wall generally remains small, the effect on dust charging would be expected to be correspondingly small. However, as dust grains – much like the wall – typically acquire a negative floating potential, they repel lower energy electrons (the majority of the population) such that only the relatively small population of high energy electrons has any impact on their charging. Removing a small fraction of electrons from the sheath (all from this high energy population, since these are also the ones with enough energy to reach the wall) therefore has a disproportionately large impact on the dust grain charge.
In this work, we consider the scenario of a capacitively-coupled RF plasma sheath with parameters corresponding to a low pressure industrial discharge, in a plasma with spatial extent $\gg$ the sheath width, so that the problem may be considered in one spatial dimension. A fluid model for electrons within the sheath is derived according to the same approach used by Nitter [55], with Poisson’s equation solved numerically to provide the sheath potential profiles. This model is then modified to account for electron-loss to the wall, and electric field-reversal within the sheath. The consequences for sheath behaviour and dust grain charging are investigated, along with the subsequent effect on the (charge-dependent) forces on dust grains in the sheath and grain motion across the sheath.

### 1.4.2 Collisions in Dust Charging

When calculating the charge acquired by a dust grain immersed in a plasma, collisions are very often neglected. This can be seen in section 1.3.1 - each of the main dust charging theories assumes conservation of angular momentum or otherwise completely neglects collisions in the vicinity of the dust grain. It is also an important assumption when the OML charging theory is derived in section 2.3 below.

This is typically justified by the fact that the dust-plasma interaction is mostly confined to within several $\lambda_{De}$ of the grain, even for a large dust grain. In the regime $\lambda_{De} \ll \lambda_{mfp}$, an often considered case [58, 59, 60, 61] (where $\lambda_{mfp}$ is the mean free path for whichever type of collision is dominant in the chosen plasma), very few incoming particles will experience a collision during their interaction with a grain. As a result, it is assumed that collisions have little effect on grain charging.

Lampe et al. [62, 63, 4], however, noted that although ions approaching from outside the grain’s potential well necessarily have positive total energy (and therefore can only collide with the grain or escape the potential well), a collision within the grain’s potential well can produce an ion with insufficient energy to escape the grain. If this ion is not absorbed by the grain, it will end up trapped on an orbital trajectory around the grain.

These orbital trajectories are notable because of their stability; unless deorbited by a further collision, such ions will remain in orbit around the dust grain indefinitely. For a plasma with sparse collisions, it may take a long time for trapped ions to build up in orbit, but it will happen. In addition, since the rates at which ions are knocked into
and out of orbiting trajectories are both proportional to the collision frequency, $\nu_{\text{coll}}$, the density of trapped ions is independent of $\nu_{\text{coll}}$ in the steady-state [64].

Lampe et al. considered charge-exchange collisions, which are often the dominant type of ion collision in industrial edge plasmas [65] and also occur in tokamak edge plasmas [66]. These occur when an ion collides with a neutral atom from the un-ionised background gas and the charge on the ion is transferred to the neutral, without energy or momentum transfer between the two particles [67]:

$$A^+ + A \rightarrow A + A^+.$$ (1.4)

While these collisions do not transfer energy between the particles involved, they may still result in the newly ionised atom having a lower energy than the initial ion, particularly if the ions are flowing relative to the neutrals or the ion temperature is greater than that of the neutral gas $T_i > T_n$. Even for cold-ion industrial plasmas with $T_i \approx T_n$, the post-collision ion is likely to have lower energy than the initial ion if the collision occurs inside the grain potential well (since the ion will have been accelerated during its interaction with the grain before the collision).

In the work of Lampe et al., they found that this mechanism allows a significant population of trapped ions to build up in orbit around a dust grain, and that this population affects the shielding of the dust potential by the surrounding plasma and the dust charging process.

The work done by Lampe et al. on this issue was carried out in a uniform, stationary plasma. Here, we investigate this effect in the strongly flowing plasma found in the plasma edge, where dust is most commonly found.

We find that the greatly increased ion flow past the dust grain increases the rate at which trapped ions are produced, significantly increasing the effect on the dust grain’s charge and potential distribution. This phenomenon is investigated via the use of a two-dimensional hybrid computational approach, allowing the 2-D structure of the potential in the plasma flow to be resolved.

While the plasma is considered to flow past the dust grain, we do not consider the dust grain moving relative to the plasma boundary. The speeds achieved by a moving dust grain are far less than the ion flow speed in the edge plasma. Thus, a non-stationary dust grain will affect the scenario under consideration only by moving between different regions of the plasma boundary, with varying external electric fields,
ion flow speeds, and and charge imbalances. This is considered an avenue of further research.

1.5 Relevance to Current Problems

For any of the applications mentioned in section 1.3 to be better investigated, fundamental dust-plasma interactions, especially dust grain charging must be better understood.

In recent work to use dust as a diagnostic to determine the extent and structure of the sheath (a useful research avenue, since traditional Langmuir probes disturb the plasma they are inserted to measure), a comparison of experiment [21] and theory [68] was carried out. The theory, which included an OML-based approach to dust grain charging with Maxwellian electrons, was able to qualitatively predict dust grain levitation height near the sheath edge, but not the minimum stable levitation position of a dust grain further inside the sheath. It was also noted that trapped ion effects had been disregarded but could play a significant role under certain conditions.

In another work to investigate the formation of dust crystals in the sheath [22], the experimentally measured dust grain charge was found to be smaller than the OML comparison could account for. In both cases, a greater understanding of the importance of different sheath effects and dust charging processes would be of value.

In industrial applications, even though dust is fairly efficiently kept from contaminating processing surfaces directly, there is an interest in dust charging due to the effect a levitating layer of negatively charged dust can have on the sheath structure. Even a low concentration of dust particles has been shown to affect the sheath width, and induce spatial oscillations into the sheath profile [69]. As a sink for incoming plasma particles, they can also affect the ion flux to the wall [70] - a crucial quantity for plasma surface etching techniques. Studying the effect of dust grains on the plasma sheath profile is therefore also of significant interest, and again dependent on the nature of the dust-plasma interaction in and around the sheath.

1.5.1 Layout of Work

In the following work, Chapter 2 covers existing theory for modelling of the sheath region of an RF-driven plasma discharge and the OML theory for charging of dust in the sheath, along with the resulting forces acting on the charged grain. Chapter 3 presents a modification to the sheath model described in Chapter 2, taking into account
the absorption of electrons at the sheath wall, and modifies the OML charging theory accordingly; Chapter 3 also describes the computational approach used to calculate the results of the improved model. In Chapter 4, the results of this model are then presented, and contrasted with the results of the Boltzmann electron model. In Chapter 5, a computational model is laid out to evaluate the effect of charge-exchange collisions on dust charging and dust-plasma interaction in a fast-flowing edge plasma. The results of this model are presented and discussed in Chapter 6, including predictions for orbiting trapped-ion populations and their shielding effect on dust grains. Lastly, in Chapter 7, the results of previous chapters are discussed and options for further work laid out.
Chapter 2

Background Theory

This chapter, a 1-D model of the planar sheath adjacent to an absorbing wall is derived, addressing the ion and electron densities within the sheath and the charge acquired by the wall.

The most commonly used dust charging theory is also derived, along with a discussion of its validity within the sheath region. The forces acting on a charged grain in the sheath are also explained. Together, these allow the motion of dust grains in the sheath to be calculated.

2.1 Particle densities within the sheath

2.1.1 Parameters and Timescales

The sheath model used in the rest of this section relies on several assumptions, the most notable being that electron inertia is negligibly low and the electrons can therefore respond to oscillations in the electrical potential much faster than the oscillation timescale.

The frequency with which electrons oscillate in response to charge imbalances or imposed fields is the ‘electron plasma frequency’:

\[ \omega_{pe} = \left( \frac{n_e e^2}{m_e \epsilon_0} \right)^{1/2} \]

Therefore, this assumption amounts to the statement that the electron plasma frequency is much greater than the oscillation frequency \( \omega_{pe} \gg \omega_{rf} \).
Similarly, the ion response to potential oscillations is assumed to be much slower than the oscillation timescale:

$$\omega_{pi} = \left( \frac{n_i e^2}{m_i e_o} \right)^{1/2} \ll \omega_{rf}. \quad (2.2)$$

If these criteria were not met, a more advanced treatment of the electron and/or ion populations would be required, taking into account the collective time-dependent response of the electrons and ions to the RF oscillation.

The plasma parameters used in this investigation were an Argon plasma, ion mass $m_i = 6.68 \times 10^{-26} \text{kg}$, with density at the sheath edge of $n_o = 1.0 \times 10^{15} \text{m}^{-3}$. This gives plasma frequencies at the sheath edge of $\omega_{pe} = 1.78 \times 10^9 \text{rad s}^{-1}$ and $\omega_{pi} = 6.59 \times 10^6 \text{rad s}^{-1}$.

In this work, potential oscillations in the sheath are caused solely by the application of an RF driving voltage to the wall. The frequency chosen was $\omega_{rf} = 8.52 \times 10^7 \text{rad s}^{-1}(= 2\pi \times 13.56 \text{MHz})$, as is common in industrial plasma experiments [23, 55, 3, 56] — comfortably within the parameter regime required for these assumptions to be valid. As such, the electrons can be modelled as responding to the instantaneous value of the sheath potential, while ions only react to its DC component [56].

Other parameters used were electron temperature $T_e = 2.3 \times 10^4 \text{K} (= 2e\text{V})$ and RF driving voltages of $0 \leq V_{rf} \leq 500\text{V}$.

### 2.1.2 Additional Assumptions

Two significant additional assumptions are made in this section. The first is that the sheath may be considered in only one spatial dimension - i.e. there are no geometric effects due to the shape or surface smoothness of the wall. This is valid for a wide variety of plasma applications, where such a smooth surface is used. These may include plasma processing surfaces for thin film deposition [71], where the smoothness of the surface is crucial to the application, and cleaning of plasma-facing surfaces such as diagnostic mirrors via applied RF fields to induce sputtering [72], as well as research to investigate dust-plasma interactions [21, 3], where a (relatively) simple sheath structure is beneficial for analysis of collected data.

In addition, this assumption may be valid for certain surfaces which are not entirely smooth, but where the scale of the surface inhomogeneities is sufficiently small, such as semiconductor chip etching plasmas in which channels of $\sim 10 - 100\text{nm}$ scale are
etched in a smooth surface [73].

However, for surfaces coated in irregularities such as dust or sputtered material re-deposited on the wall, the charging of such material is significantly different to the planar wall [74], and the sheath structure is likely to be also if the inhomogeneities are comparable in scale to $\lambda_{De}$. An additional case where the 1D sheath approximation is likely invalid is that of RF antennas in contact with plasmas [75], since the shape of the antenna surface is highly structured and will introduce significant additional complexities to the sheath modelling.

The second assumption is the use of the two-scale model, which results both in a set of boundary conditions for the sheath (i.e. an asymptotic sheath edge where the electric field fades to zero) and, consequently, in the Bohm criterion for ion speed discussed below. At the typical pressures given in section 1.2.2 (and assuming a neutral gas temperature of 300K and collision cross-section $\approx 3 \times 10^{-19}$m$^2$ [55]), the ion-mean free path, $\lambda_{mfp}$, is between 0.7 - 140mm (2 - 415 $\lambda_{De}$, for the plasma parameters given in the previous section).

Since the presheath width is often $\sim \lambda_{mfp}$, the two-scale model will be invalid at higher pressures, and ions will be accelerated towards the boundary in a single edge region without clear distinction between 'sheath' and 'presheath' regions, as quasineutrality will break down smoothly over the whole region. However, for lower pressures, $\lambda_{mfp} \gg \lambda_{De}$ and the two-scale approximation remains valid. We choose to assume a low-pressure regime here, and for simplicity, use the two-scale model.

Intermediate pressures could also be addressed, however, by simply altering the sheath model to take into account ion-collisions within the sheath and allowing for a non-zero electrostatic field at the sheath-edge [55], and could be of interest for future work.

2.1.3 Ions

In the two-scale theory, ions are accelerated from the bulk plasma towards the sheath by an electrostatic field in the quasi-neutral presheath region. Assuming the ions are cold relative to the electrons – commonly true for industrial plasma applications [76] – it can be shown that in the two-scale limit ($\lambda_D/\lambda_i \to 0$), at the point where quasineutrality breaks down, ions must be traveling at or above a minimum speed, the Bohm Speed, equal to the ion acoustic speed. A full derivation of this criterion can be found
A further analysis [16, 13] shows that in the same limit, the ion speed in the presheath is limited to \( v_i \leq v_B \). As a result, at the sheath edge (the boundary between sheath and presheath, where quasi-neutrality breaks down), the ion speed at the sheath edge must equal the Bohm speed, making the sheath edge a sonic barrier.

Within the sheath, ions are attracted to the wall by the sheath electrostatic field. Thus, ion density is governed by the 1-D continuity equation and energy conservation equations:

\[
 n_i(x) v_i(x) = n_o v_B \tag{2.4}
\]

\[
 \frac{1}{2} m_i v_i(x)^2 + e \Phi_{dc}(x) = \frac{1}{2} m_i v_B^2 \tag{2.5}
\]

where \( n_i \) is ion density, \( v_i \) is ion speed, \( e \) is the magnitude of the electronic charge, \( \Phi_{dc} \) is the DC sheath potential (relative to the sheath edge where \( \Phi = 0 \)), and the x-coordinate is the direction along which ions flow (perpendicular to the wall); the background neutral gas density is taken to be sufficiently low that ion-neutral collisions can be neglected, and we consider only positive, singly charged ions.

Combining equations 2.4 and 2.5 gives the ion number density within the sheath:

\[
 \tilde{n}_i = \left(1 - 2 \tilde{\Phi}_{dc}\right)^{-1/2} \tag{2.6}
\]

where \( \tilde{n} = n/n_o \) is the normalised ion density relative to the density at the sheath edge and the DC potential has been normalised to \( \tilde{\Phi}_{dc} = e \Phi_{dc}/(k_B T_e) \); \( k_B \) is Boltzmann’s constant.

## 2.1.4 Electrons

We assume that electrons in the central plasma, far from the walls, are in thermal equilibrium and thus described by a Maxwell-Boltzmann velocity distribution as they enter the sheath, following the approach of Nitter (1996) [55]:

\[
 v_i \geq v_B = \sqrt{\frac{k_B T_e}{m_i}}. \tag{2.3}
\]
\[ f(v_{eo}) = \beta \exp \left( -\frac{m_e v_{eo}^2}{2k_BT_e} \right) \] (2.7)

where \( v_{eo} \) is the speed (perpendicular to the wall) of an electron at the sheath edge, and \( \beta = n_o \sqrt{m_e / (2\pi k_B T_e)} \) is a normalising constant, to set \( n_e = n_o \) at the sheath edge. This Maxwell-Boltzmann distribution is also assumed to have negligible bulk flow towards the wall due to the relatively high thermal motion of electrons, and the repulsive nature of the negatively charged wall.

Electron energy conservation gives the electron speed deeper in the sheath, relative to its speed at the sheath edge:

\[ \frac{1}{2} m_e v_{ex}^2 (x) - e\Phi(x) = \frac{1}{2} m_e v_{eo}^2 \] (2.8)

where \( v_{ex} \) is the speed perpendicular to the wall of an electron (initially moving at speed \( v_{eo} \) as it entered the sheath), \( m_e \) is the electron mass, and \( \Phi \) is the instantaneous sheath potential. A phase-space mapping from the sheath edge using Liouville’s theorem [77] then gives the distribution function within the sheath:

\[ f(v_{ex}, \Phi) = f(v_{eo}) = \beta \exp \left( -\frac{m_e v_{eo}^2}{2k_BT_e} \right) \] (2.9)

\[ f(v_{ex}, \Phi) = \beta \exp \left( \frac{2e\Phi(x) - m_e v_{ex}^2}{2k_BT_e} \right). \] (2.10)

Integrating over velocity space gives the electron density – a Boltzmann distribution, as is commonly used in sheath modelling:

\[ \tilde{n}_e(x,t) = \frac{1}{n_o} \int_{-\infty}^{\infty} f(v_{ex}, \Phi) dv_{ex} = \exp \left( \Phi(x,t) \right). \] (2.11)

The ion and electron densities (as a function of potential) are shown in figure 2.1. As can be seen, the ion density decreases (due to conservation of ion flux) as the ions are accelerated into the negative sheath potential, but electron density decreases even more rapidly - leading to the positive space charge sheath discussed in Chapter 1.

### 2.1.4.1 Maxwell-Boltzmann Distribution

In his work, Nitter recognised that in truth, the plasma near the sheath edge is unlikely to be in thermal equilibrium, and the electron velocity distribution may be made up
of several populations, with none of these being strictly Maxwellian. Often, the distribution in an RF-driven plasma may be bi-Maxwellian (made up of two Maxwellian distributions with different temperatures) [76, 78].

However, the Boltzmann relation is commonly used to model electron densities and, as seen above, it is closely related to the Maxwellian distribution. Since the main aim of Chapters 3 and 4 is to investigate the (typically neglected) loss of electrons to the plasma-edge wall, we retain the Maxwellian assumption in order to allow direct comparison of sheath profiles and dust charging with and without consideration of electron loss.

The use of a single Maxwellian distribution may also be considered a step towards applying the approach from Chapter 3 to a bi-Maxwellian velocity distribution.

![Figure 2.1](image-url)  
Figure 2.1: Ion and electron densities as a function of potential (equations 2.6 and 2.11 respectively).
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2.2 Wall Charging

If the potential of the wall is not externally set via a DC driving voltage, the wall reaches a steady-state when it has charged sufficiently negatively that the electron flux is reduced to match the ion flux to the wall.

If the plasma is driven by a capacitively-coupled RF voltage applied to the wall, this does not provide an additional source of net current to the wall [25]. The sinusoidal driving voltage $V_{rf}$ is therefore imposed on top of the floating potential of the wall $V_{dc}$, which is still determined by time-averaged electron and ion current balance:

$$V_{\text{wall}}(t) = V_{dc} + V_{rf} \cos(\omega_{rf} t)$$  \hspace{1cm} (2.12)

where $f_{rf} = \omega_{rf} / (2\pi)$ is the RF driving frequency.

We assume that the wall provides a perfectly absorbing surface for incident electrons and ions, with negligible reflection or secondary electron emission, as these effects primarily occur at higher energies than those considered here [79].

The resulting ion current density to the wall, $J_i$, is then:

$$J_i = e n_o v_B. \hspace{1cm} (2.13)$$

This does not depend on the wall potential since the ion flow is entirely anisotropic (all ions are considered to be flowing towards the wall), and the wall potential only accelerates them in this direction while (as discussed in section 2.1.3) total ion flux remains constant.

The electron current, however, does depend on the wall potential, since the sheath field tends to repel electrons from the wall; consequently, the electron current varies over the RF cycle. The electron current is found by taking the first moment of the electron velocity distribution to find the one-way electron flux at the wall:

$$\langle J_e(t) \rangle = \left\langle -e \int_{-\infty}^{0} v f(v_{ex}, \Phi = V_{\text{wall}}) dv_{ex} \right\rangle \hspace{1cm} (2.14)$$

where $\langle J_e \rangle$ denotes the time-averaged electron current density to the wall.

The Maxwellian electron distribution function (equation 2.9) gives:
\[
\langle J_e \rangle = -e n_o \frac{v_t e}{\sqrt{2\pi}} \exp \left( \frac{e V_{\text{wall}}(t)}{k_B T_e} \right) \tag{2.15}
\]

where \(v_t e = \sqrt{k_B T_e / m_e}\) is the electron thermal speed. Applying equation 2.12 for \(V_{\text{wall}}(t)\), and time-averaging over the RF cycle, this becomes:

\[
\langle J_e \rangle = -e n_o \frac{v_t e}{\sqrt{2\pi}} \exp \left( \frac{e V_{dc}}{k_B T_e} \right) I_o \left( \frac{e V_{rf}}{k_B T_e} \right) \tag{2.16}
\]

where \(I_o\) is a zeroth-order modified Bessel function.

By combining equations 2.13 & 2.15 under the condition of time-averaged current balance, \(\langle J_e \rangle + J_i = 0\), it is possible to determine the DC component of the wall potential [55]:

\[
\tilde{V}_{dc} = \frac{1}{2} \ln \left( \frac{2\pi m_e}{m_i} \right) - \ln \left( I_o \left( \tilde{V}_{rf} \right) \right) \tag{2.17}
\]

where \(V_{dc}\) and \(V_{rf}\) have been normalised to \(\tilde{V} = eV / (k_B T_e)\). This result is shown in figure 2.2, where it can be seen that for increasing \(\tilde{V}_{rf}\), the DC wall potential becomes more negative at almost the same rate as the applied \(\tilde{V}_{rf}\) increases. In fact, the rate of change, \(d\tilde{V}_{dc} / d\tilde{V}_{rf} < 1\) (marginally), and the oscillation component of the wall potential slowly approaches the same magnitude as the time-averaged component as greater \(\tilde{V}_{rf}\) is applied.
2.3 Dust Charging

To calculate the charge acquired by dust in the sheath, we considered individual spherical dust grains which, like the sheath wall, absorb incident plasma particles without reflection or secondary emission. Grains with radii \( r_d \approx 5 \times 10^{-6} \) \( \mu \text{m} \) were considered.

For small dust grains in the sheath, \( r_d \ll \lambda_{De} \), dust charging processes are often considered independently from sheath effects by assuming that the dust-plasma interaction occurs on a scale far smaller than any sheath gradients. In this work, Orbital Motion Limited (OML) theory is applied to calculate the charge acquired by the dust grain, using the plasma conditions local to the dust’s position in the sheath and ignoring...
density and speed gradients in the vicinity of the dust, as well as the external sheath field. The limits to this approach are discussed in section 2.3.2.

2.3.1 Orbital Motion Limited Theory

The most commonly used dust charging theory is the Orbital Motion Limited approach. By considering particles approaching the grain from outside the potential well with various impact parameters, the OML approach attempts to calculate the impact parameter at which a grazing collision with the grain will occur (figure 2.3). The derivation of Shukla and Mamun [27] is followed here:

OML assumes conservation of energy and angular momentum in the central potential surrounding the charged dust grain.

\[
\frac{1}{2} m_j v_o^2 = \frac{1}{2} m_j v_g^2 + q_j \phi_d \quad (2.18)
\]

\[
m_j v_o b_{\text{crit}} = m_j v_g r_d \quad (2.19)
\]

where \(m_j\) and \(q_j\) denote the mass and charge of a plasma particle of species \(j\) (ion or electron), \(\phi_d\) is the surface potential of the dust grain (relative to the local plasma just
outside the grain’s potential well), $b_{\text{crit}}$ is the impact parameter of a particle approaching the grain with an initial speed $v_o$ and reaching a speed $v_g$ at its closest point of approach to the grain (as shown in figure 2.3).

Combining equations 2.18 and 2.19 gives the critical impact parameter for a particle-grain collision, and hence the collision cross-section $\sigma_d$:

$$b_{\text{crit}} = r_d \sqrt{1 - \frac{2q_j \phi_d}{m_j v_o^2}} \quad (2.20)$$

$$\sigma_d^j = \pi b_{\text{crit}}^2 = \pi r_d^2 \left(1 - \frac{2q_j \phi_d}{m_j v_o^2}\right). \quad (2.21)$$

For a 3-dimensional velocity distribution $f_j(v_o)$ far from the dust grain, the current to the grain can then be calculated as:

$$I_j(\phi_d) = \int \int q_j v_o \sigma_d^j(v_o, \phi_d) f_j(v_o) \, d^3v_o \quad (2.22)$$

where $I_j$ is the current to the grain from species $j$ with dust-collision cross-section $\sigma_d^j$ and 3-dimensional distribution function $f_j(v, \phi)$.

In the sheath case of monoenergetic ions, this simply becomes:

$$I_i(\phi_d) = n_o e \pi r_d^2 v_B \left(1 + \frac{2\tilde{\phi}_d}{2\Phi_{\text{dc}}(x) - 1}\right) \quad \text{for} \quad e\phi_d < \frac{1}{2}m_i v_B^2 - e\Phi_{\text{dc}} \quad (2.23)$$

$$I_i = 0 \quad \text{for} \quad e\phi_d \geq \frac{1}{2}m_i v_B^2 - e\Phi_{\text{dc}}$$

where $\phi_d$ has been normalised to $\tilde{\phi}_d = e\phi_d/(k_B T_e)$ and $\Phi_{\text{dc}}(x)$ is the normalised DC sheath potential at the dust grain’s position. As before, the ion current responds to the local DC sheath potential $\Phi_{\text{dc}}$, rather than oscillating with the instantaneous sheath potential $\Phi(x,t)$. Equation 2.23 is derived in full in Appendix A.

In the case of a complete 3-dimensional Maxwellian distribution of electrons in the sheath (equation 2.9), the electron current to the grain is [55]:

$$I_e = -n_o e \pi r_d^2 \sqrt{\frac{8k_B T_e}{\pi m_e}} \exp \left(\tilde{\Phi}(x,t) + \tilde{\phi}_d\right) \quad \text{for} \quad \tilde{\phi}_d \leq 0 \quad (2.24)$$
\[ I_e = -n_0 e \pi r_d^2 \sqrt{\frac{8 k_B T_e}{\pi m_e}} \exp \left( \Phi(x,t) \right) \left( 1 + \hat{\phi}_d \right) \text{ for } \hat{\phi}_d > 0. \] (2.25)

The equation changes form for \( \phi_d < 0 \) since the negative dust repels incoming electrons and there is a minimum speed \( v_{\text{min}} = \sqrt{2e\phi_d/m_e} \) required for electrons to reach the grain. Equations 2.24 and 2.25 are also derived in full in Appendix A.

The charging time for a dust grain is significantly longer than an RF oscillation - Nitter [55] calculated the charging time for a 10 \( \mu \)m dust grain as several \( \mu \)s while the RF time period is 74ns. Consequently, the oscillation of the dust charge over an RF timescale is not considered. As with the sheath wall, the steady-state potential of a dust grain is then calculated by DC electron and ion current balance

\[ \langle I_e(\phi_d, \Phi(x,t)) \rangle + I_i(\phi_d, \Phi_{dc}(x)) = 0. \] (2.26)

The solution to this current-balance equation is found numerically, and (for small dust grains, \( r_d \ll \lambda_{De} \)) can be related to the charge on the grain, \( Q_d \), via the vacuum capacitance of a sphere:

\[ Q_d = 4\pi e_0 r_d \phi_d. \] (2.27)

Since the solution to equation 2.26 at a particular position \( x \) in the sheath depends on the shape and amplitude of the oscillation of \( \Phi(x,t) \) around its time-averaged value \( \Phi_{dc}(x) \), this is complex to evaluate and varies for different RF driving amplitudes \( \tilde{V}_{rf} \). However, using the numerical approach detailed below in section 2.5, the solution \( \phi_d(\Phi_{dc}) \) is shown for various sheath profiles in figure 2.4.
2.3.2 OML Limitations and Accuracy

2.3.2.1 Validity of OML Assumptions

The OML theory relies on several assumptions which limit its validity, particularly within the sheath. These are:

1. Conservation of energy
2. Conservation of angular momentum
3. A homogeneous and isotropic plasma surrounding the grain
4. The existence of a grazing trajectory

Each of these criteria is broken in the sheath to some degree. However, they can be satisfied if the dust grain is small compared to relevant length scales.

Figure 2.4: OML equation (2.26) solved for various RF sheaths.
Conservation of energy requires that the work done by the sheath field over this scale, $W_s$, is small compared to the work done by the dust’s electric field $W_d \approx q_d \phi_d$.

Assuming the dust-plasma interaction is approximately confined to within $9 r_d$ of the grain’s surface (where the dust field has dropped to 1% of its surface value) and taking a typical sheath field $E_s \approx \frac{k_B T_e}{e \lambda_{De}}$:

$$W_s = 9 r_d e E_s \approx 9 r_d q_d \frac{k_B T_e}{e \lambda_{De}}.$$  \hfill (2.28)

Comparing this to a dust grain potential $\phi_d \approx -3 \frac{k_B T_e}{e}$ (which can be seen in figure 2.4 and the supplementary figure given in Appendix B to be a typical value):

$$\left| \frac{W_s}{W_d} \right| = 3 r_d \lambda_{De} \ll 1.$$  \hfill (2.29)

The plasma parameters in Chapter 2 give a Debye length $\lambda_{De} = 332 \mu m$; for a 5$\mu m$ dust grain, this work-ratio is then $\approx 0.045$.

This calculation assumes a particle approaches the grain directly along the axis of the sheath field. This may be accurate for ions, but will not be for electrons which may approach from any angle. For any other angle of approach, the work done will be reduced. As such this represents the maximum possible value for the work done by the sheath and the average effect on an incoming electrons will in fact be even smaller.

Conservation of energy also relies on collisions being sparse over the dust scale. Since these simulations are being carried out for a collisionless sheath with $\lambda_{De} \ll \lambda_{mfp}$, and the dust grains being considered are much smaller than the Debye length, $r_d \ll \lambda_{De}$, this condition can be considered well met.

Since the grain field is radial and exerts no torque on incoming particles, conservation of angular momentum requires that the angular momentum imparted to an incoming particle by the sheath field, $\Delta L$, is small compared to its initial angular momentum $L_o$:

$$\Delta L = \int_{r_d}^{10 r_d} \frac{\tau}{v_r} dr = \int_{r_d}^{10 r_d} \frac{q_j r E_s \sin(\theta)}{v_r} dr$$  \hfill (2.30)

where $\tau$ is the torque from the sheath field $E_s$, $v_r$ is the particle’s radial speed, and $\theta$ is the angle (about the dust grain) between the particle and the sheath-field axis.
If the potential well around the grain varies as $\phi(r) = \phi_d r^d/r$, then radial speed is given by conservation of energy and angular momentum to be:

$$v_r(r) = v_o \sqrt{1 - \frac{2q_d \phi_d r^d}{mv_o^2 r} - \left(\frac{b_{\text{crit}}}{r}\right)^2}.$$  \hfill (2.31)

For a grazing-incidence particle, with initial angular momentum of $L_o = mv_o b_{\text{crit}}$:

$$\frac{\Delta L}{L_o} = \frac{q_j E_s \sin(\theta)}{mv_o b_{\text{crit}}} \int_{r_d}^{10r_d} \frac{r}{v_r} dr.$$  \hfill (2.32)

A (highly crude) simplifying assumption has been made that the particle’s trajectory to the grain has constant $\theta$, as otherwise it is necessary to numerically solve for the particle’s complete trajectory towards the grain. That will be done in section 2.3.2.2, however for the purposes of the analytic approach in this section, it is a necessary assumption.

For an ion at speed approaching with an initial speed $v_o = v_B$ with $\sin \theta = b_{\text{crit}}/(10r_d)$, and $\phi_d \approx -3k_B T_e/e$ and $E_s \approx k_B T_e/e \lambda_{De}$, this integral can be numerically calculated as:

$$\frac{\left|\Delta L\right|}{L_o} \approx 3.76 \frac{r_d}{\lambda_{De}}.$$  \hfill (2.33)

This evaluates to $\approx 0.057$ for $\lambda_{De} = 332 \mu$m and a $5 \mu$m grain.

For an electron approaching the same grain with an initial speed $v_o = 3.5v_{te}$ (electrons with speeds less than $\sim 2.5v_{te}$ cannot overcome the grain’s potential barrier and have no collision cross-section), and taking $\sin \theta = 1$ so that the electron approaches perpendicular to the sheath field:

$$\frac{\left|\Delta L\right|}{L_o} \approx 6.09 \frac{r_d}{\lambda_{De}}.$$  \hfill (2.34)

This evaluates to $\approx 0.092$. However, again this overestimates the effect on an average incoming electron as most do not approach the grain directly perpendicular to the sheath field.

The assumption of isotropy in the plasma surrounding the dust grain is broken in the sheath due to the density and speed gradients across the sheath. However, the spatial scale on which particle speeds and densities vary in the sheath, $\lambda_{De}$, is much larger than the radius of the dust-plasma interaction ($\sim 10r_d$) and is consequently neglected.
Neglecting any small density gradients on the dust scale is further justified when calculating the electron current to the grain by the fact that any density gradient across the grain will produce both an increased electron current from the higher density side and a reduced current from the lower density side, partially cancelling its effect. In the ion case, conservation of ion flux in the sheath removes any explicit dependence on the local ion density from the ion-current expression (equation 2.23).

The dust grain also tends to focus the ion flow directly behind it, creating a beam of increased density ions and therefore a non-isotropic surrounding plasma. However, as long as $r_d \ll \lambda_{De}$, there is insufficient ion charge in this region to significantly distort the shape of the grain’s potential well and therefore this ion wake should have little impact on grain charging.

Finally, OML assumes that a trajectory is possible which grazes the dust grain surface and then escapes. This is not often true as an absorption radius can exist for ions [80], greater than the grain radius, such that trajectories passing within this absorption radius will inevitably hit the grain. This effect occurs as a result of the distribution of space-charge formed by the plasma surrounding the grain; if this space-charge is sufficient to cause the potential surrounding the grain to vary more steeply than $1/r^2$, an absorption radius will exist rendering the OML approach invalid [48].

However, for monoenergetic ions, it has been shown that as $r_d/\lambda_{De}\rightarrow 0$, no absorption radius exists and the OML result becomes valid [80]. In addition, Kennedy and Allen [48] showed that for ion temperatures as low as $T_i = 0.01T_e$, the $\phi_d$ obtained using OML converged with the result of the full Orbital Motion theory for dust grains with radius $r_d \lesssim 0.1\lambda_{De}$.

Other charging processes may also occur, such as secondary electron emission when ions collide with the grain, or thermionic emission from a hot dust grain. However, these are not considered here as they are typically secondary effects and are also not directly relevant to the processes being investigated.

### 2.3.2.2 Numerical Error Estimate

In addition to the analysis done above, numerical work was carried out to estimate the effect of the sheath field on the accuracy of the OML approach. Ion trajectories were numerically integrated under imposed electrostatic fields, to find the critical impact
parameter $b_{\text{crit}}$ numerically and compare it to the OML value.

To do this, the sheath electrostatic field was calculated for a DC sheath (with no RF driving voltage) by integrating Poisson’s equation:

$$
\frac{\partial^2 \tilde{\Phi}(x)}{\partial \tilde{x}^2} = \tilde{n}_e \left( \tilde{\Phi}(x) \right) - \tilde{n}_i \left( \tilde{\Phi}(x) \right)
$$

(2.35)

where potential and density have been normalised to $\tilde{\Phi} = e\phi/(k_B T_e)$ and $\tilde{n} = n/n_o$ as before, and position is normalised to $x = x/\lambda_{De}$.

Using the equations for ion and electron density (2.6 and 2.11), Poisson’s equation can be integrated once analytically to give:

$$
\frac{1}{\sqrt{2}} \frac{\partial \tilde{\Phi}(x)}{\partial \tilde{x}} = \sqrt{\exp \left( \tilde{\Phi} \right) + \sqrt{1 - 2\tilde{\Phi}}} - 2.
$$

(2.36)

See appendix A for a full derivation of equation 2.36. This must then be integrated again numerically to find the spatial profile for the sheath potential, $\Phi(x)$, in the vicinity of the grain, and the electrostatic field $E_s(x)$.

On top of the sheath field, an unshielded radial field $E_r(r) = \phi_d e / r^2$ was imposed, centered on the dust grain. This approximation is imperfect, since the dust grain field will distort the ion (and electron) densities in the vicinity of the grain. However, for a small dust grain, $r_d \ll \lambda_{De}$, the sheath field is close to linear over the scale of the dust-plasma interaction and the field around the grain is approximately unshielded over most of its range. Any perturbation due to the interaction of the two fields is therefore neglected in this error estimate.

Ions were initialised at a position $200r_d$ upstream of the grain with an impact parameter $b$: $x_{\text{init}} - x_{\text{grain}} = (200r_d, b)$. The initial ion velocity, $v_{\text{init}} = (-\sqrt{v_o^2 - 2e\Delta\Phi/m_i}, 0)$, is given by ion energy conservation, reducing the ion’s initial speed to the value it would have $200r_d$ closer to the sheath edge.

$$
v_o = v_B \sqrt{1 - 2\Phi_{dc}}
$$

is the ion speed found in the OML approach - the speed an ion would have at the grain’s position, under the sole influence of the sheath field - and $\Delta\Phi$ is the potential difference between this position and the ion’s starting location.

$$
\Delta\Phi = -\int_{x=0}^{200r_d} E_s dx.
$$
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Figure 2.5: Ion trajectories with various initial impact parameters and constant $v_o = 3v_B$, moving under sheath and dust electrostatic fields.

The ion trajectory was then tracked under a force $\vec{F} = e(E_r (r) \sin \theta - E_s, E_r (r) \cos \theta)$ (the sum of the sheath field $E_s$ and grain field $E_r (r) = \phi_d r^2/r^2$), with the integration carried out by an implicit Adams-Moulton method (detailed in section 5.2.3).

Thus, the ion is accelerated up to speed $v_o$ as it approaches the grain, while simultaneously interacting with the sheath potential - unlike the OML approach, which separates the two processes and assumes an ion approaches the grain pre-accelerated to $v_o$ before its interaction with the grain.

Ion trajectories were repeatedly integrated, altering the impact parameter $b$, until the critical impact parameter $b_{\text{crit}}$ was found numerically. This method is shown in figure 2.5, which shows ions with different initial impact parameters moving under the imposed force $\vec{F}$. A grain charged to $\phi_d = -3k_B T_e/e$ was used for these simulations.

The critical impact parameters found using this method are shown in figures 2.6 and 2.7, which compare the numerically determined $b_{\text{crit}}$ with the OML prediction for varying ion speeds.
Figure 2.6: Numerically calculated critical impact parameter for ions compared to the OML prediction from equation 2.21, for varying ion speed.

Figure 2.7: Numerically calculated critical impact parameter for ions, $b_{\text{crit}}$, as a fraction of the OML prediction $b_{\text{oml}}$, from equation 2.21, for varying ion speed.
Figure 2.8: Numerically calculated critical impact parameter for ions, $b_{\text{crit}}$, as a fraction of the OML prediction, $b_{\text{oml}}$, from equation 2.21, for varying grain potential.

It is notable that the error estimate given via this approach is significantly lower than the approximations in section 2.3.1. This is because the energy and angular momentum imparted by the sheath field to a particle as it approaches the grain are not strictly ignored in the OML approach, but effectively applied before the OML calculation is carried out. In this numerical approach, the dust-plasma interaction region is simply expanded to its true extent, while OML assumes the interaction occurs over an infinitesimally small distance compared to the sheath scale.

It can also be seen that the significance of both sheath and grain fields decreases rapidly as $v_o$ increases, such that for high ion speeds, $b_{\text{crit}} \rightarrow r_d$ and the collision cross-section becomes the grain’s geometric cross-section.

The error estimate increases as the dust potential $\phi_d$ is increased. This is to be expected, as it increases the scale over which the dust interacts with incoming particles. However, even for low ion speeds, a highly negative grain is required for the error to become large. Figure 2.8 shows the error for varying $\phi_d$ and an ion speed of $v_o = 3v_B$. 
2.4 Grain Forces

A charged dust grain in the sheath is also subject to various forces acting on it. Often the dominant force is electrostatic, from the charged dust grain being in the presence of the sheath electric field. Since the timescales for grain motion and charging are both much greater than an RF period, this force is simply the result of the DC electric field:

$$F_x = Q_d E_{dc} = 4\pi \varepsilon_0 r_d \phi_d E_{dc} \hat{x}$$  \hspace{1cm} (2.37)

where $Q_d = C \phi_d$ is the dust grain charge, $C$ is the vacuum capacitance of a sphere, $\varepsilon_0$ is the permittivity of free space, $\hat{x}$ is the unit vector in the x-direction, and $E_{dc} = -\partial \Phi_{dc}/\partial x$ is the local DC sheath electric field.

Another significant force on the grain is gravity. The sheath wall here is considered to be the lower electrode of a plasma, such that the gravitational force is directed towards the wall

$$F_g = -\frac{4}{3} \pi r_d^3 \rho_d g \hat{x}$$  \hspace{1cm} (2.38)

where $g$ is acceleration due to gravity and $\rho_d$ is the dust density. A density $\rho_d = 1510$ kg m$^{-3}$ was used when calculating $F_g$; this corresponds to the material melamine formaldehyde, which is often used in dust-plasma experiments [25].

Another, usually smaller, force is ion drag. The flow of ions from the sheath edge towards the wall exerts a force on the dust grain both via direct collisions (which also charge up the grain) and via indirect Coulomb collisions. The forms of these two components are derived separately in [81], giving the ion drag force due solely to Coulomb collisions:

$$F_{id, coul} = -\frac{2\pi r_d^2 n_i e^2 \phi_d^2}{m_i v_i^2} \ln \Lambda \hat{x}$$  \hspace{1cm} (2.39)

$$\Lambda = \frac{\lambda_D^2 \left( \frac{n_e}{n_i} \right)^2 + r_d^2 \left( \frac{e \phi_d}{m_i v_i} \right)^2}{r_d^2 \left( 1 - \frac{e \phi_d}{m_i v_i^2} \right)}$$  \hspace{1cm} (2.40)

and the force due to impact-collisions:

$$F_{id, coll} = -\pi r_d^2 m_i n_i v_i^2 \left( 1 - \frac{2e \phi_d}{m_i v_i^2} \right) \hat{x}$$  \hspace{1cm} (2.41)
where \( n_i \) and \( v_i \) are the local ion density and speed respectively. In both cases when calculating the ion drag force, it is assumed that the dust grain speed relative to the wall is negligible compared to the ion flow speed.

Since industrial plasmas are often only partially ionised, there is also a background neutral gas present. If the grain is moving relative to this gas, it will encounter an additional drag force exerted by this neutral gas. We assume a gas of constant temperature, with no bulk flow relative to the wall. We also assume that incident gas atoms colliding undergo a diffuse reflection on collision [82]. This gives the ‘Epstein expression’ for neutral drag [83, 55]:

\[
F_{\text{neut}} = -\frac{16}{3}\sqrt{\pi}r_d n_{\text{neut}} k_B T_n \left( 1 + \frac{\pi}{8} \right) \frac{v_{\text{dust}}}{v_{\text{th}}} \hat{v}_{\text{dust}}.
\]

(2.42)

Other forces may also be considered, such as a thermophoretic force due to neutral gas temperature gradient. However, under the sheath conditions considered here, those listed above are typically the dominant forces [84, 52].

2.5 Numerical Approach

Since \( \omega_{pe} \ll \omega_{rf} \ll \omega_{pe} \), electron density is only a function of instantaneous potential \( \Phi (x, t) \) and the ion density is a function of the time-averaged potential \( \Phi_{dc} = \langle \Phi (x, t) \rangle \). As neither species is therefore explicitly time-dependent, the potential \( \Phi (x, t) \) can easily be built from multiple instantaneous solutions \( \Phi (x, t_i) \) to Poisson’s equation at various times throughout the RF oscillation, where \( t_i \) is one of \( N \) time points chosen from \( 0 \leq \omega_{rf} t_i < 2\pi \)

\[
\frac{\partial^2 \Phi (x, t_i)}{\partial \tilde{x}^2} = \tilde{n}_e \left( \tilde{\Phi} (x, t_i) \right) - \tilde{n}_i \left( \tilde{\Phi}_{dc} (x) \right).
\]

(2.43)

The wall boundary condition \( V_{\text{wall}} (t_i) = V_{dc} + V_{rf} \sin (\omega_{rf} t_i) \) is applied (using \( V_{dc} \) from equation 2.17), while the second boundary condition is an asymptotic approach to the reference potential \( \Phi (x \rightarrow \infty, t_i) = 0 \) as per the two-scale theory [12, 85]. Potential and density are normalised as before, while the distance from the wall, \( x \), is normalised to the electron Debye length at the sheath edge: \( \tilde{x} = x/\lambda_{De} \).

A shooting method approach was taken to the boundary value problem of solving for \( \Phi (x, t_i) \). This involved numerically integrating from the wall towards the plasma, using
a fourth order Runge-Kutta integrator \cite{86} to integrate equation 2.43. Since only one boundary condition at the wall is known, $V_{\text{wall}}(t)$, an approximate guess for $\frac{\partial \Phi}{\partial x}|_{x=0}$ was used as the second initial condition for the integration. The value for this initial gradient was then altered, repeating the integration, until the asymptotic sheath-edge condition was met.

As the form of $\tilde{\Phi}_{dc}(x) = \langle \Phi(x,t) \rangle$ is not initially known, an approximate solution is chosen, so that the instantaneous solutions $\Phi(x,t_i)$ can be calculated via numerical integration. The approximate solution used was the potential profile from 2.36, which can easily be numerically integrated with a single boundary condition ($\Phi|_{x=0} = V_{dc}$) to give $\tilde{\Phi}_{dc}^{(0)}(x)$, the initial guess for the DC sheath profile.

Once all the instantaneous solutions were calculated, they were averaged to provide an improved estimate for $\tilde{\Phi}_{dc}(x)$, and the process was iterated until $\tilde{\Phi}_{dc}(x)$ converged:

$$\tilde{\Phi}^{(j)}(x,t_i) = \int \tilde{n}_e \left( \tilde{\Phi} \right) - \tilde{n}_i \left( \tilde{\Phi}_{dc}^{(j)}(x) \right) \, dx^2 \quad (2.44)$$

$$\tilde{\Phi}_{dc}^{(j+1)}(x) = \langle \Phi^{(j)}(x,t) \rangle \quad (2.45)$$

where the superscripts $j$ and $j+1$ denote increasing iteration number.

To ensure convergence in the shooting method approach, we use the increasing monotonic relationship between the initial gradient, $\frac{\partial \Phi}{\partial x}|_{x=0}$, and the potential at the far edge of the integration region. When ‘shooting’ different initial gradients to find the correct value, the value was altered by increments of size $\lesssim 0.5 \frac{\partial \Phi}{\partial x}|_{x=0}$. When an increment was found that caused the potential at the far edge of the integration region to change sign, it was known that in this interval was the correct initial condition.

An interval bisection approach was then used to find its value, with $\geq 20$ iterations. This ensured that the initial gradient was accurate to $< 1$ in $2^{20}$.

Once the sheath potential profile is known, it is a simple matter to evaluate the OML potential on dust grains in the sheath by matching the ion and electron currents (section 2.3.1), and then to also evaluate the forces acting on those dust grains (section 2.4).
Chapter 3

Improved Electron Model

The Boltzmann model described in the previous chapter offers a fundamental contradiction, in that an electron current is drawn by the wall (to match the completely anisotropic ion current), but the electrons are assumed to be in thermal equilibrium, and electron losses to the wall are ignored when calculating other aspects of the sheath, such as the electron density profile and current to dust grains within the sheath.

Electron absorption by the wall in fact leads to a non-isotropic velocity distribution function, which affects the space-charge in the sheath region, the charging of the wall, and the charging of dust grains within the sheath.

The contradiction in the Boltzmann model becomes a greater problem at higher RF driving voltages, when a non-monotonic form to the sheath potential can develop at the peak of the RF oscillation. In this case, the sheath field transiently reverses direction close to the wall. Electrons in this region are consequently accelerated towards the plasma boundary during the field reversal - a fundamentally non-equilibrium situation.

Kinetic models of the sheath are capable of simulating electron dynamics self-consistently and accounting for electron loss to the wall, but do so at significant computational cost - and still do not offer an easy analytic approach to calculating the electron current to dust grains within the sheath.

In this chapter, for the first time to the author’s knowledge, a (relatively) simple fluid model is derived, which provides a self-consistent approach to calculating electron densities and electrostatic fields within the sheath, and the OML dust charging model is modified to take into account this altered electron velocity distribution.
3.1 Electron Velocity Distribution

An electron moving towards the wall at some point in the sheath, a distance $x$ from the wall, can overcome the sheath potential barrier and reach the wall if its speed exceeds:

$$v_{\text{cut}}'(x, t) = \sqrt{2e(\Phi(x, t) - V_{\text{wall}})} / m_e$$  \hspace{1cm} (3.1)

where $V_{\text{wall}}(t) = \Phi|_{x=0,t}$ is the instantaneous potential at the wall.

Since all electrons enter the sheath from the plasma side (none are considered to be emitted from the wall), any electron moving in the positive x-direction (away from the wall - see figure 3.1) is one which has been reflected in the sheath potential. As a result, no electrons with $v_{\text{ex}} > v_{\text{cut}}'$ will return towards the plasma as they will instead reach the wall. Therefore, the velocity distribution will not be a complete Maxwellian, but will instead be cut off above a certain point [17, 55].

This is shown in figure 3.1, which gives the electron velocity distribution function at two points in a sheath. Far from the wall, most electrons do not have sufficient energy to overcome the potential barrier and $v_{\text{cut}}'$ is large. However, closer to the wall, the potential barrier to overcome is smaller and $v_{\text{cut}}'$ shrinks correspondingly to remove a significant fraction of the distribution.

Since the timescale for electron-electron Coulomb collisions in this plasma is $\tau_{ee} \approx 40\mu s$ [87], far longer than either the RF oscillation timescale (74ns) or the electron transit time across the sheath ($2\pi\omega_{pe}^{-1} = 0.56\text{ns}$), electrons are not able to re-thermalise their velocity distribution via collisions within the sheath.
Figure 3.1: Instantaneous sheath potential profile at $\omega_{rf} t = 0$, the peak of the RF oscillation, for sheath with driving voltage $V_{rf} = 25k_B T_e/e$; local electron distribution function inset, for two positions in the sheath.

The blue-shaded section of the distribution indicates electrons with insufficient energy to reach the wall, while red-shading indicates electrons with sufficient energy to reach the wall. The red-shaded section on the left corresponds to the missing electrons on the right-hand side of the distribution.

The $x$ coordinate perpendicular to the wall has been normalised to the electron Debye length: $x = x/\lambda_D$, and electron speed has been normalised to the electron thermal speed $\bar{v} = v/v_{th}$.

The resultant velocity distribution is therefore able to remain anisotropic, and is given by:

$$f(v_{ex}, \Phi, V_{wall}) = \alpha' \exp \left( \frac{2e\Phi(x) - m_e v_{ex}^2(x)}{2k_B T_e} \right) \text{ for } v_{ex} < v'_{cut}$$
where \( \alpha' = 2\beta/F'_o \) is a normalising factor for the new distribution. The electron number density can be obtained by integrating this distribution:

\[
 n_e = \int_{-\infty}^{v_{\text{cut}}} f(v_{\text{ex}}, \Phi, V_{\text{wall}}) \, dv_{\text{ex}}.
\]

Carrying out this integral, we obtain a normalised number density

\[
 \tilde{n}_e = \exp \left( \tilde{\Phi}(x) \right) \left( 1 + \text{erf} \left( \frac{\tilde{v}_{\text{cut}}}{\sqrt{2}} \right) \right) / F'_o
\]

where \( F'_o = \left( 1 + \text{erf} \left( \sqrt{-V_{\text{wall}}} \right) \right) \) is a normalising factor to set \( \tilde{n}_e = 1 \) at the sheath edge.

As this new density only departs noticeably from the Boltzmann result when \( \Phi - V_{\text{wall}} \lesssim k_B T_e/e \), and the potential typically increases rapidly away from the wall, this change is often confined to a narrow region close to the wall where \( n_e \ll n_i \) anyway, rendering its effects negligible even here. This can be seen clearly in figure 3.2.

Figure 3.2a shows the potential profile for a DC sheath (with no applied RF driving voltage) increasing steeply near the wall. 3.2b shows the relative ion and electron densities, with \( n_e \ll n_i \) near the wall. 3.2c shows the electron density from this new cutoff model (equation 3.3) as a fraction of the electron density predicted by a Boltzmann model (equation 2.10), with the ratio of the two only departing from equality close to the wall.

However, in an RF driven sheath, the situation may be different. An RF driving voltage applied to the wall at the plasma edge causes the potential within the sheath to oscillate. At the minimum of the RF oscillation (and through most of the rest of the cycle) the factors keeping the cutoff correction negligible remain in effect. Around the peak of the RF cycle, though, the sheath potential is small and increases shallowly away from the wall value, causing the cutoff effect to extend far into the sheath. At this time also, \( n_e \approx n_i \) through much of the sheath, such that the impact of the cutoff on the sheath potential is greatly magnified.

These effects are shown in figure 3.3. An RF sheath potential profile is evaluated
at $\omega_{rf}t = 0$ and $\omega_{rf}t = \pi$, the peak and trough of the RF cycle respectively. The resulting electron density variation can be seen in 3.3b, with the electron density even lower at $\omega_{rf}t = \pi$ but approximately equal to the ion density at $\omega_{rf}t = \pi$. Figure 3.3c then shows the spatial variation of the cutoff correction at these times, with the effect extending far into the sheath at the peak of the RF cycle.

It should be noted that this electron effect has no significant impact on the Bohm speed since the latter, being an ion quantity, is related to the time-averaged electron density $\langle n_e \rangle$ and near the sheath edge this remains very close to Boltzmann (both because the effect in question occurs for a relatively short proportion of the time and because it diminishes towards the sheath edge).
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Figure 3.2: Spatial profiles for floating DC sheath ($\hat{V}_{rf} = 0$).

Figure 3.3: Spatial profiles for an RF driven sheath (driving voltage $\hat{V}_{rf} = 30$).
3.1.1 Wall charging

Re-evaluating equation 2.14 for this new electron velocity distribution gives a modified electron current density to the wall:

$$\langle J_e \rangle = -en_o v_e \sqrt{\frac{m_e}{2\pi}} \exp\left(\frac{eV_{\text{wall}}(t)}{k_B T_e} \right) \left. \frac{2}{F_o'(t)} \right).$$  (3.4)

For a large wall potential, $|\tilde{V}_{\text{wall}}| > 1$, the term $2/F_o'(t) \to 1$ quickly, and $J_e$ returns to the expression in Chapter 2.

Equating the time-averaged ion and electron currents in this case, $\langle J_e \rangle + J_i = 0$, gives:

$$\left\langle \exp\left(\tilde{V}_{\text{dc}} + \tilde{V}_{rf} \sin(\omega_{rf} t)\right)\middle/ F_o'\left(\tilde{V}_{\text{dc}} + \tilde{V}_{rf} \sin(\omega_{rf} t)\right) \right\rangle = \sqrt{\frac{\pi m_e}{2 m_i}}.$$  (3.5)

In this case, there is no simple analytic expression, and a solution for $\tilde{V}_{\text{dc}}$ must be found numerically.

3.2 Field reversal

As can be seen from equation 2.17, the magnitude of $V_{\text{dc}}$ monotonically increases with increasing $V_{rf}$. Since an increased potential drop across the sheath implies a faster ion flow speed at the wall, this causes progressively lower ion densities in the vicinity of the wall (due to conservation of ion flux) as the driving voltage is increased.
More negative wall potentials also decrease electron density. However, the change in $V_{dc}$ from applying an RF voltage $V_{rf}$ is smaller than $V_{rf}$ itself, such that the voltage oscillation on the wall grows relative to its average value and the peak wall potential $V_{dc} + V_{rf}$ is in fact a monotonically increasing function of the driving voltage. This can be seen in figure 3.4. Consequently, the peak electron density at the wall is also a monotonically increasing function of $V_{rf}$.

The result of this is that around the peak of the RF cycle, the electron density briefly exceeds the ion density near the wall (shown in figure 3.5), leading to two oppositely charged layers in the sheath. When this effect becomes sufficiently large, it causes the electric field to reverse within the wall-side layer, causing electrons in this region to be attracted towards the wall rather than repelled during the RF peak.

Rather than increasing monotonically from the wall to the sheath edge, as shown earlier in figures 3.1 - 3.3, the resulting sheath potential profile has a minimum within the sheath below the level of the wall potential, $\Phi_{\text{min}}(t) < V_{\text{wall}}(t)$. This effectively acts as the new loss-point for electrons instead of the wall, since any electron passing this point will definitely reach the wall.

The electron velocity distribution is therefore altered during a field-reversal, taking the form:
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Figure 3.5: Ion density and peak electron density (evaluated using the Boltzmann model) at the wall with increasing $V_{rf}$.

\[
f(v_{ex}, \Phi, \Phi_{min}) = \frac{2\beta}{F_o} \exp \left( \frac{2e\Phi(x,t) - m_e v_{ex}^2(x)}{2k_B T_e} \right) \text{ for } v_{ex} \leq v_{cut} \tag{3.6}
\]

\[
f(v_{ex}, \Phi, \Phi_{min}) = 0 \text{ for } v_{ex} > v_{cut}. \tag{3.7}
\]

This is largely the same as the velocity distribution function from equation 3.2, except that $F_o = \left( 1 + \text{erf} \left( \sqrt{-\Phi_{min}(t)} \right) \right)$ is evaluated at the potential minimum rather than the wall (where $\Phi_{min}(t)$ is the minimum value of the instantaneous sheath potential $\Phi(x,t)$).

In addition, the form of $v_{cut}$ is slightly altered:

\[
v_{cut}(x) = \sqrt{2e(\Phi(x) - \Phi_{min})/m_e} \left| \frac{\partial \Phi}{\partial x} \right| \tag{3.8}
\]

In the positively charged layer away from the wall, $\partial \Phi/\partial x \geq 0$ and the cutoff velocity remains positive. $v_{cut}$ reaches zero at the potential minimum (since electrons reaching this point will experience no further potential barrier in reaching the wall).

In the negatively-charged layer close to the wall, $v_{cut}$ is negative, representing the fact that electrons will have increasingly negative speeds as they are accelerated towards the wall in this region. Velocity distributions for both inside and outside the field-reversed...
The electron density during a field-reversal can be found by integrating the distribution function, as before, giving:

\[ \tilde{n}_e = \exp\left(\tilde{\Phi}(x)\right) \left(1 + \text{erf}\left(\frac{\tilde{v}_{\text{cut}}}{\sqrt{2}}\right)\right) / F_o. \] (3.9)

As noted by Valentini [57], the Boltzmann relation becomes completely invalid in this region.

Electron density decreases between the field-reversal point and the wall, as electrons crossing the potential minimum are accelerated towards the wall. In the Boltzmann model, however, \( \tilde{n}_e \) is only a function of the instantaneous potential, \( \tilde{\Phi} \); consequently, the increasing potential approaching the wall would be taken to imply an increasing electron density. This represents a fundamentally different prediction between the two models, which is investigated in Chapter 4.
Figure 3.6: Sheath potential profile with field reversal ($\tilde{V}_{ef} = 100$), with electron distribution function inset both inside and outside field-reversal region.
Blue-shaded section of the distribution indicates electrons with insufficient energy to reach the wall; red-shading indicates electrons with sufficient energy to reach the wall ($|v_{ex}| > v_{cut}$).
Since the red-shaded electrons have sufficient energy to reach the wall, there are no returning electrons with $v_{ex} > v_{cut}$ on the right hand side of the distribution.
In the field-reversed region, all electrons will reach the wall as they are now in an attractive potential rather than a repulsive one.

3.2.1 Wall-charging with field reversal

Since the effect of the field reversal is to increase the potential barrier to the wall, fewer electrons reach the wall. This results in an excess ion current to the wall, and the DC wall potential becomes more positive than expected from equation 2.17 to re-balance the currents.
As electron current to the wall is now a function of $\Phi_{\text{min}}(t)$, and no longer an explicit function of $V_{\text{wall}}(t)$ – though the potential minimum remains a function of the
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wall potential – calculating the DC wall potential becomes more complicated in the case of a field-reversal.

Section 3.4 explains how an iterative approach is used to find both $\Phi_{\text{min}}(t)$ and $V_{\text{wall}}(t)$.

3.3 Dust Charging

In the case of an incomplete Maxwellian velocity distribution (equation 3.2), evaluating the OML integral (equation 2.22) is more complicated, with three equations describing the electron current to the grain (rather than two, as in Chapter 2). The first of these, 3.10, is derived in full in appendix A. The others can be derived in exactly the same manner, but with different limits on the integration.

In the case of a positively charged grain:

$$I_e = -I_{eo} \left[ \left(1 + \tilde{\phi}_d\right) - \frac{1}{2} \left(1 + \tilde{\phi}_d\right) \exp\left(-\frac{\tilde{v}_{\text{cut}}^2}{2}\right) + \tilde{v}_{\text{cut}} \sqrt{\frac{\pi}{8}} \left(\frac{1}{2} + \tilde{\phi}_d\right) \text{erfc}\left(\frac{\tilde{v}_{\text{cut}}}{\sqrt{2}}\right) \right] \frac{2}{F_o}$$

(3.10)

where $I_{eo} = n_e e \pi r_d^2 \sqrt{\frac{8k_B T_e}{\pi m_e}} \exp\left(\tilde{\Phi}(t)\right)$, which does not depend on the dust grain potential, has been condensed for simplicity, and $\tilde{v}_{\text{cut}}$ is evaluated at the dust grain’s location within the sheath.

Comparing equation 3.10 to the Maxwellian OML charging equation for a positive dust grain, equation 2.25,

$$I_e = -I_{eo} \left(1 + \tilde{\phi}_d\right)$$

one can see the increased complexity of this new form for the electron current. The $\left(1 + \tilde{\phi}_d\right)$ term remains, and the subsequent terms are corrections due to the altered electron distribution. While it is difficult to isolate an exact meaning for each term, the second term can perhaps be understood as a linear correction to the current due to the missing portion of the electron distribution; the third term arises due to geometric effects, since the cutoff is not an isotropic effect in velocity space (a similar calculation with an isotropic cutoff in velocity space does not give rise to an error function term).

It can be seen that, as $\tilde{v}_{\text{cut}} \to \infty$, both additional terms tend to zero, and for a complete Maxwellian distribution the electron current is restored to its original form.
In the case where $\tilde{v}_{\text{cut}} = 0$ (i.e. next to the wall, where exactly half the Maxwellian distribution is missing), the third term again tends to zero, the angular dependence being far simpler in this scenario; the second term becomes $\frac{1}{2}$ the base current, leading to a 50% drop in electron current - exactly as would be expected with half the distribution missing relative to the standard formula.

In the case of a negatively charged grain, there is a minimum initial electron speed, $v_{\text{min}} = \sqrt{2e\phi_d/m_e}$, for incident electrons to collide with the grain.

If $v_{\text{min}} < v_{\text{cut}}$, the electron current is given by:

$$I_e = -I_{eo} \left[ \exp \left( \tilde{v}_d \right) - \frac{1}{2} \exp \left( -\frac{\tilde{v}_{\text{cut}}^2}{2} \right) \left( 1 + \tilde{v}_d \right) + \tilde{v}_{\text{cut}} \sqrt{\frac{\pi}{8}} \left( \frac{1}{2} + \tilde{\phi}_d \right) \text{erfc} \left( \frac{\tilde{v}_{\text{cut}}}{\sqrt{2}} \right) \right] \frac{2}{F_o}$$  \hspace{1cm} (3.11)

and if $v_{\text{min}} > v_{\text{cut}}$:

$$I_e = -I_{eo} \left[ \left( \frac{1}{2} + \frac{\tilde{v}_{\text{cut}} v_{\text{min}}}{4} \right) \exp \left( \tilde{v}_d \right) + \frac{\tilde{v}_{\text{cut}}}{\sqrt{8}} \left( \frac{1}{2} + \tilde{\phi}_d \right) \text{erfc} \left( \frac{\tilde{v}_{\text{min}}}{\sqrt{2}} \right) \right] \frac{2}{F_o}. \hspace{1cm} (3.12)$$

We can again compare these to the Maxwellian OML current for a negatively charged grain, equation 2.24,

$$I_e = -I_{eo} \exp \left( \tilde{v}_d \right).$$

In equation 3.11, it can be seen that the exponential term $\exp \left( \tilde{v}_d \right)$ remains intact, and the same additional terms are included as in equation 3.10 to account for the missing section of the distribution; however, in 3.12, the initial exponential term is modified. This is because physically the $\exp \left( \tilde{\phi}_d \right)$ term represents the fact that as a grain becomes more negative, low energy electrons are increasingly unable to overcome its repulsive potential and reach the grain (to contribute to the charging current). The cutoff, however, is an effect occurring for high energy electrons (above $v_{\text{cut}}$). Thus, in equation 3.11 the two effects appear separately - the exponential term remains intact and the same cutoff terms as eqn 3.10 are superimposed on the end.

In equation 3.12, the cutoff has come to low enough energies that $v_{\text{min}} > v_{\text{cut}}$; since the negative grain potential affects incoming electrons with speed $v < v_{\text{min}}$ and the cutoff removes electrons with speed $v > v_{\text{cut}}$, these two now overlap in the region
\( v_{\text{min}} > v > v_{\text{cut}} \), creating a more complex scenario in which individual terms are hard to interpret.

In both cases, the Maxwellian OML result is recovered for \( \tilde{v}_{\text{cut}} \to \infty \). In equation 3.12, the \( \tilde{v}_{\text{cut}} = 0 \) result also reduces to half of the Maxwellian OML current, as expected. For 3.11, it is required that \( v_{\text{min}} < v_{\text{cut}} \), so the \( \tilde{v}_{\text{cut}} = 0 \) result reduces to half the Maxwellian current under the condition that \( v_{\text{min}} = 0 \) also.

In addition, a further two cases must be considered in order to describe the electron current during the field-reversal, as the electrons are being accelerated towards the wall, shifting the electron distribution function to higher energies.

For the electron distribution function (equation 3.6) within the reversed electric field \( (E > 0) \) region, when \( \tilde{\phi}_d \geq 0 \) or only slightly negative \((\tilde{\phi}_d < 0 \text{ but } v_{\text{min}} \leq v_{\text{cut}})\):

\[
I_e = -I_{eo} \left[ \frac{1}{2} \exp \left( -\frac{\tilde{v}_{\text{cut}}^2}{2} \right) \left( 1 + \tilde{\phi}_d \right) - \tilde{v}_{\text{cut}} \sqrt{\frac{\pi}{8}} \left( \frac{1}{2} + \tilde{\phi}_d \right) \text{erfc} \left( \frac{\tilde{v}_{\text{cut}}}{\sqrt{2}} \right) \right] 2/F_o \tag{3.13}
\]

while for larger negative grain potentials \((\tilde{\phi}_d < 0 \text{ and } v_{\text{min}} > v_{\text{cut}})\):

\[
I_e = -I_{eo} \left[ \left( \frac{1}{2} - \frac{\tilde{v}_{\text{cut}} v_{\text{min}}}{4} \right) \exp \left( \tilde{\phi}_d \right) - \tilde{v}_{\text{cut}} \sqrt{\frac{\pi}{8}} \left( \frac{1}{2} + \tilde{\phi}_d \right) \text{erfc} \left( \frac{\tilde{v}_{\text{min}}}{\sqrt{2}} \right) \right] 2/F_o \tag{3.14}
\]

These two cases bear similar terms to the above equations, but are hard to compare directly to the Maxwellian OML case since the entire distribution is being accelerated towards the wall (as shown in figure 3.6), and an even greater degree of anisotropy is therefore present than in equations 3.10-3.12.

The dust grain charging time is much greater than the RF time period, so by calculating the instantaneous electron current \( I_e(t) \) across an RF cycle, and equating the time-averaged current to the ion current, one can find the steady-state dust grain charge.

Since the form of the electron current changes for different \( \phi_d \) regimes (and also across the RF cycle as the sheath potential, and hence \( v_{\text{cut}}, \) varies), the grain charge cannot be calculated analytically and must be solved numerically.
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3.4 Numerical Approach

The numerical approach used to evaluate this model largely follows that of section 2.5, though with a several extra factors which increase the computational complexity.

As before, Poisson’s equation is solved numerically at various times $t_i$ throughout the RF cycle, with boundary conditions $V_{\text{wall}}(t_i) = V_{dc} + V_{rf} \sin(\omega_{rf} t_i)$ at the wall and $\Phi(x \to \infty, t_i) = 0$ far from the wall. In this case, $V_{dc}$ is given by the more complicated expression in equation 3.5 which must be solved numerically.

The most significant complicating feature in this new model is that when $V_{rf}$ is high enough to induce a field reversal, $n_e$ becomes a function of $\Phi_{\text{min}}$:

$$\frac{\partial^2 \Phi(x, t_i)}{\partial x^2} = \tilde{n}_e \left( \Phi(x, t_i), \tilde{\Phi}_{\text{min}}(t_i) \right) - \tilde{n}_i \left( \tilde{\Phi}_{dc}(x) \right). \quad (3.15)$$

This required a further level of iteration in solving for each $\Phi(x, t_i)$, since the position and value of $\Phi_{\text{min}}$ cannot be known in advance of knowing the entire potential profile. To solve for each instantaneous potential $\tilde{\Phi}(x, t_i)$, an initial guess for $\tilde{\Phi}_{\text{min}}^{(0)} = \tilde{V}_{\text{wall}}$ was made. This was used to integrate Poisson’s equation using the shooting method described in section 2.5, providing an initial estimate of the potential profile $\tilde{\Phi}^{(0)}(x, t_i)$.

$$\tilde{\Phi}^{(0)}(x, t_i) = \int \tilde{n}_e \left( \Phi(x, t_i), \tilde{\Phi}^{(0)}_{\text{min}}(t_i) \right) - \tilde{n}_i \left( \tilde{\Phi}_{dc}(x) \right) dx^2. \quad (3.16)$$

This potential profile a new value $\tilde{\Phi}_{\text{min}}^{(1)} = \min \left[ \tilde{\Phi}^{(0)}(x, t_i) \right]$, which is an overestimate of the magnitude of the field-reversal, since any field reversal $\tilde{\Phi}_{\text{min}} < \tilde{V}_{\text{wall}}$ decreases the electron density, giving a smaller field-reversal effect. Thus, this provides a search interval in which to find the self-consistent value of $\tilde{\Phi}_{\text{min}}$ using interval bisection.

The other computational complexity introduced by the field reversal is the altered DC wall charging, resulting from $\Phi_{\text{min}}(t) < V_{\text{wall}}(t)$. To solve this, each time a new DC sheath profile was constructed, equation 3.5 was evaluated at $\Phi_{\text{min}}(t)$ rather than $V_{\text{wall}}(t)$:

$$\left\langle \exp \left( \tilde{\Phi}_{\text{min}}(t) / F'_o \tilde{\Phi}_{\text{min}}(t) \right) \right\rangle = \sqrt{\frac{\pi m_e}{2m_i}}. \quad (3.17)$$

The variable $\tilde{V}_{\text{dc}}^{i+1}(t) = \tilde{\Phi}_{\text{min}}^{i+1}(t) - \tilde{V}_{\text{dc}}^i$ was substituted in to allow an improved estimate $\tilde{V}_{\text{dc}}^{i+1}$ to be evaluated:
\[
\exp\left(\tilde{V}_{\text{dc}}^{i+1}\right) \exp\left(\Phi^i_{\text{diff}}(t) / F_o' \Phi^i_{\text{min}}(t)\right) = \sqrt{\frac{\pi m_e}{2m_i}}. \tag{3.18}
\]

This approach assumes the temporal profile of \(\Phi_{\text{diff}}(t)\) does not change significantly for small changes in \(\tilde{V}_{\text{dc}}\). Since the field reversal is a secondary charging effect for the wall, only occurring for large \(V_{\text{rf}}\) where this voltage is the dominant factor in determining the wall potential barrier, this approach was found to be accurate.

These equations are evaluated in the next chapter to give sheath potential profiles for various RF driving voltages, and the results of this model compared and contrasted with the earlier Boltzmann electron model.

It is worth noting that, while the derivations in this chapter have been carried out for a truncated Maxwell-Boltzmann distribution (both for simplicity and for more direct comparison with the Boltzmann thermal equilibrium model), the same approach can in principle be followed for a bi-Maxwellian velocity distribution \([76, 78]\), or indeed any of a range of electron velocity distributions sometimes found in the sheath. The work carried out in this chapter can therefore be used as a template for a wider variety of calculations than just a truncated Maxwellian - and has scope beyond that directly demonstrated in this work.
Chapter 4

Results

In this chapter, the commonly used sheath and dust charging models from Chapter 2 are compared to the improved electron models derived in Chapter 3. The effects on both sheath profiles and dust charging are investigated, and significant differences noted between the two models.

The plasma parameters given in section 2.1 were used, with varying driving voltages $V_{\text{rf}}$. A spatial resolution of $0.01\lambda_{De}$ was used when calculating $\Phi(x,t_i)$, and 25 time points $t_i$ distributed across the RF cycle. As discussed in Chapter 2, the spatial sheath profiles are integrated using a fourth order Runge-Kutta integration scheme. Taking $\lambda_{De}$ as the natural length-scale of the problem, the Runge-Kutta integration (with global truncation error $O(h^4)$), gives individual $\Phi(x,t_i)$ accurate to $O(10^{-8})$ for this spatial step size.

Since $V_{\text{wall}}$ varies perfectly sinusoidally, the temporal resolution may seem excessive; however, within the sheath, the nonlinear response of electrons to the imposed RF oscillation causes the potential to vary non-sinusoidally as higher frequency harmonics are generated in $\Phi(x,t)$ away from the wall. The potential profile $\Phi(t)$ is shown in figure 4.1 for several RF driving voltages at a set position within the sheath, demonstrating this effect.

Thus, a greater temporal resolution is necessary to accurately determine potential profiles near the peak of the RF oscillation. Typically, probes inserted into the plasma (passing through an RF sheath) require at least the first and second harmonics of the RF oscillation (as well as the fundamental frequency) to be compensated for, in order to achieve accurate measurements [25, 88]. The temporal resolution used here allows
up to the twelfth harmonic to be resolved, so should be more than sufficient. To ensure that the temporal resolution was sufficient in these simulations, Fourier transforms of the oscillation were taken to inspect the harmonic generation (figure 4.2). As noted in experiments, the first and second harmonics were significant, while no harmonics higher than the 4th ($\omega = 5\omega_{rf}$) were found to be appreciable at any point. Thus, the temporal resolution used can accurately resolve the important oscillatory properties of this sheath.

From this point onward, the Boltzmann electron model from Chapter 2 will be referred to using the abbreviation BE, and abbreviation CC will be used for the cutoff-corrected model derived in Chapter 3. This is done for ease of graph annotation, and clarity.

4.1 Sheath potential

As $V_{rf}$ is increased, the standard wall-charging formula (equation 2.17) with the BE model produces peak potential profiles which increasingly differ from when the CC model is used and the altered wall potential due to the field reversal is correctly accounted for in the wall-charging calculation.

This can be seen in figure 4.3 which compares the peak potential profiles predicted by the BE and CC models. The wall voltage and shape of the potential profile during the RF peak both diverge for higher driving voltages. It is also of note that the CC model delays the onset of the electric field reversal compared to the BE case and predicts a lower-magnitude field reversal at higher $V_{rf}$.

Figure 4.3 also demonstrates that after the field-reversal occurs, the wall charging is affected as predicted in section 3.2, with the wall potential becoming more positive than expected from the BE model. Figure 4.4 shows the rate at which the peak wall potential increases, compared to the old-wall charging formula, earlier shown in figure 3.4.

As a result of this correction, it can be seen that the peak wall potential $V_{dc} + V_{rf}$ becomes positive around $\tilde{V}_{rf} = 210$ rather than the $\sim 1850$ initially predicted.
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Figure 4.1: Temporal profile of sheath oscillation at $\hat{x} = 10\lambda_{De}$ from the wall, for various RF driving voltages. Dashed lines indicate perfectly sinusoidal profile without higher harmonics. These particular oscillation profiles are generated using the CC model.

Figure 4.2: Fourier transform of sheath oscillation showing amplitude of higher harmonics generated in the sheath. This transform was taken at $\hat{x} = 10\lambda_{De}$ for $\hat{V}_{rf} = 100$. 
This effect occurs because the BE model does not accurately treat the lower electron current to the wall after the onset of the field-reversal. While the CC model predicts a higher potential at the wall, electron density at the wall in the CC model is primarily a result of $\Phi_{\text{min}}$, the minimum point in the instantaneous potential profile, as any electrons passing this point will reach the wall.

As a result, even though the potential at the wall is higher, the peak electron current at the wall is lower than predicted by the BE model. Figure 4.5 shows how the magnitude of the electron current density to the wall at $\omega_{rf}t = 0$ varies with driving voltage.

It can also be seen in figure 4.5 that a positively charged wall ($\tilde{V}_{rf} > 210$) does not cause a runaway increase in electron current to the wall. In a sheath with a monotonically varying potential, a positively charged wall cannot be maintained since (as discussed in Chapter 1), the sheath forms in order to decrease electron current to the wall to equal the ion flux. In a sheath with a non-monotonically varying potential, however, the potential barrier between the plasma and the wall can exist despite the positive charge on the wall, since an electron must have sufficient energy to pass the potential minimum $\Phi_{\text{min}}$ before it ‘sees’ the attractive field of the positively charged wall.
Figure 4.4: Peak $V_{\text{wall}}$ prediction based on equation 2.17 (BE model) along with the actual peak wall potential from the cutoff model (CC) with field-reversal accounted for.

The importance of the region around the potential peak can be seen in figure 4.6. The electron current profile to the wall is shown to become progressively narrower and more sharply peaked with greater RF driving voltages. For high $V_{rf}$, the electron current to the wall is dominated by a narrow time window around $\omega_{rf}t = 0$ (the peak wall voltage), making the sheath potential around this time, both its size and spatial profile, a key factor in determining electron dynamics in the sheath over the whole RF cycle.

4.2 Dust grain results

The electron current to dust grains in the sheath becomes similarly peaked with increasing $V_{rf}$, such that the sheath potential profile around the RF peak is key to calculating the dust grain charge in the interior of the sheath. This is shown in figure 4.7, which applies the CC model to calculate the grain potential $\phi_d$ within the sheath, and compares it to that obtained from the BE model. It can be seen that in the inner sheath, the $\phi_d \text{CC}$ is significantly smaller than $\phi_d \text{BE}$ and this effect extends further into the sheath for increasing $\tilde{V}_{rf}$. 
As the field-reversal increases for higher driving voltages, the grain potential predicted by the CC model, $\phi_{d, CC}$, becomes progressively smaller close to the wall and for sufficiently high $V_{rf}$ the grain can become positively charged. This is shown in figure 4.8.

Both figures 4.7 and 4.8 apply for a complete range of dust radii, as the grain potential predicted by OML theory does not explicitly depend on the grain radius (assuming $r_d$ remains $\ll \lambda_{De}$ in order for the underlying OML assumptions to remain valid). While the dust grain potentials predicted by the two models are only shown in ratio here, they are provided separately in Appendix B, for additional context.

Since the electrostatic force is one of the dominant forces on micron-scale dust in the sheath, this effect on the dust grain charge translates directly into an effect on the forces it experiences and the type of motion it undergoes in the sheath.
Figure 4.6: Magnitude of the normalised electron current density $\tilde{J}_e = J_e / (#n_vte)$ at the wall, varying over an RF cycle. The current becomes progressively more peaked at $\omega_{rf}t = 0$ as $V_{rf}$ is increased.

In figure 4.9, for a moderate $V_{rf}$, the total force (the sum of the forces listed in section 2.4) acting on a dust grain can be seen to differ by up to a factor of 4 in the inner sheath when BE and CC models are compared. The forces are broken down by component (electrostatic, ion drag, and gravitational) in Appendix B, for further information.

Figure 4.10 shows a higher driving voltage where shape of the force profile differs significantly between the two models. In the CC model, the force on the dust grain is negative throughout the inner sheath, while it is always positive in the BE model. In both figures 4.9 and 4.10, the forces are evaluated for a stationary grain and so neutral drag is neglected.
These significantly different force profiles lead to altered dust grain trajectories within the sheath. Figures 4.11 and 4.12 show identical (10μm) dust grains entering the sheath with various initial velocities. These trajectories were obtained using a fourth order Runge-Kutta integrator to numerically integrate the dust trajectories once the sheath potential profiles and force profiles above were calculated. The charge on each dust grain (and consequently the forces acting on the grain) was allowed to evolve over time using the two different charging models. Neutral drag force is also included in obtaining these results, with $n_{\text{neutral}} = 1.6 \times 10^{21} \text{m}^{-3}$ and $T_n = 300 \text{K}$; any mass change due to the ion flux to the dust grain is, however, neglected as it is assumed to be negligible for the timescales and dust grain sizes under consideration.

Figure 4.11 compares the trajectories of dust grains launched from the wall using the CC model and the BE model. Dust grains launched from the wall with the same initial velocities are shown to have drastically different trajectories within the sheath depending on the model used. It can be seen that in some cases, the outcome of the trajectory is even affected - with the two models providing different answers as to whether the grain returns to hit the wall or escapes to the sheath edge.

Figure 4.12 compares the trajectories of dust grains launched from approximately
Figure 4.8: Cutoff dust grain potentials ($\phi_{dCC}$) compared to Boltzmann electron potentials ($\phi_{dBE}$) for high $V_{rf}$.

The sheath edge. In this case, it can be seen that a grain must enter the sheath with a significantly greater speed to reach the wall, if the BE model is used.

The force-profiles for the dust grains in figures 4.11 and 4.12 are given in Appendix B, as it may be of some interest for understanding the specific trajectory differences noted here.

As the RF driving voltage is decreased, predicted dust grain motion becomes more similar between the two models. However, differences remain between the BE and CC models, even for low $V_{rf}$. This is shown in figure 4.13, which shows the trajectories of 5$\mu$m dust grains approaching the wall from the sheath edge.
Figure 4.9: Normalised force \( \tilde{F} = F \lambda_{De} / (k_B T_e) \) exerted on a 5 \( \mu m \) dust grain in the RF sheath (\( \tilde{V}_{rf} = 50 \)) for BE and CC models (denoted by solid and dashed lines respectively).

Figure 4.10: Normalised force exerted on a 10 \( \mu m \) dust grain in the RF sheath (\( \tilde{V}_{rf} = 250 \)) for BE and CC models (denoted by solid and dashed lines respectively).
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Figure 4.11: Trajectories of 10 μm dust grains, launched with various initial speeds $v_{\text{dust}}$ from the wall into an RF sheath with $V_{rf} = 200$. Dashed lines indicate results from the CC model, while solid lines are results from the BE model for the same speeds. Initial dust grain speeds $v_{\text{dust}}$ have been normalised to the Bohm speed; for reference, $v_{\text{dust}} = 10^{-5}$ equates to approximately 2.2 cm s$^{-1}$.

Figure 4.12: Trajectories of 10 μm dust grains, launched with various initial speeds from approximately the sheath edge into an RF sheath with $V_{rf} = 200$. Dashed lines indicate results from the CC model, while solid lines are results from the BE model for the same speeds.
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Figure 4.13: Trajectories of 5 μm dust grains, launched with various initial speeds from approximately the sheath edge into an RF sheath with $\tilde{V}_{rf} = 50$. Dashed lines indicate results from the CC model, while solid lines are results from the BE model for the same speeds.

4.3 Discussion

In this chapter, the effect of electron loss to the sheath wall, and consequently the inadequacy of the BE model in certain RF driven sheaths, have both been clearly demonstrated for a range of different RF driving voltages. The BE model incorrectly predicts both the charging of the wall and the shape of the peak potential within the sheath during the field-reversal. This is important because the electron current to the wall is dominated by this period of the RF oscillation.

This can be seen in the charging of dust grains by the CC model variant on OML. For higher $V_{rf}$, the dust grain potential near the wall becomes progressively smaller compared to the BE model, with this effect extending progressively further into the sheath. Eventually, the charge on the grain changes sign for high $V_{rf}$ due to the much lower electron density near the wall in the CC model (as also indicated in figure 4.5), and the consequently lower electron current to the dust grain, which allows the grain to gain a net positive charge due to the still high ion current. These effects translate
into a significant change in the forces acting on the dust grain, and its resultant motion in the sheath.

Comparing to recent external work, it is particularly noteworthy is that in experiments carried out by Sharma et al. [22] to study dust crystals, the experimentally-measured dust grain charge was found to be significantly smaller than a standard OML approach could account for - in agreement with the predictions of the CC model in this chapter.

In another experimental work by Douglass et al. [68, 21] to use dust as a sheath diagnostic, an OML-based model found good agreement with experiment in predicting dust levitation heights near the sheath edge but only qualitative agreement further inside the sheath - the same region where CC model and BE models differ.

These both suggest that the CC model has potential beyond the theoretical, and a full experimental comparison may be of significant interest.

As well as the specific applications already mentioned, this improved grain charging model would have implications on any dust-plasma interactions within the sheath, since the charging of dust is a fundamental process in determining its interactions with the plasma. The relevance would also extend beyond direct dust-plasma interaction studies, into industrial contexts where a plasma sheath has a dust component of interest (as mentioned in more detail in section 1.5).
Chapter 5

Trapped Ion Theory

This Chapter considers the effect of collisions on dust grain charging in the strong ion flow at the plasma boundary. We introduce previous work by Lampe et al. in more detail, and describe the model used here.

5.1 Introduction

The work of Lampe et al. established that in a stationary, uniform plasma, sparse collisions ($\lambda_{mfp} \gg \lambda_{De, r_d}$) can play a surprisingly significant role in the interaction between small dust grains and the plasma if the background neutral temperature and ion temperature are significantly less than the electron temperature ($T_n \approx T_i \ll T_e$). In the case of a low-temperature, partially-ionised plasma, charge-exchange is the dominant ion-collision mechanism [65]. Elastic ion-neutral collisions also occur, but present a far less efficient mechanism for production of low kinetic-energy ions.

While only a small fraction of ions passing a dust grain experience a collision during their interaction with the grain, the so-called ‘trapped ions’ which result (ions with insufficient kinetic energy to escape the dust grain’s potential well) can persist in orbital motion around the grain until deorbited by a subsequent collisions (which, for a large $\lambda_{mfp}$, are also rare events). In this manner, trapped ions may slowly build up in orbit around a grain despite the rarity of collisions, and thus contribute to shielding the charge on the grain. Figure 5.1 is reproduced from Lampe et al. [4] and shows the total space-charge within a radius $r$ of a dust grain, broken down by the source of the space-charge. $Q_e$ and $Q_u$ is represent space-charge due to electrons and untrapped ions,
respectively; $Q_i$ is trapped ion charge. As can be seen, $Q_i$ is a significant contributor to shielding the charge on the dust grain. In the figure, these charges are normalised to the grain charge.

![Graph](image-url)

Figure 5.1: Total space-charge within a radius $r$ of the dust grain, separated by source (trapped ions, untrapped ions, and electrons), normalised to the charge on the dust grain. Reproduced from Lampe et al. [4] with slight adaptation.

$r_d/\lambda_{De} = 0.015$ and $T_i = 0.017T_e$; $r - r_d$ is distance from the dust grain’s surface. $Q_u$ and $Q_e$ are the total ion and electron space charge between the grain surface and radius $r$ due to their density increase/decrease near the grain; $Q_i$ is the total trapped ion charge within radius $r$.

While they affect the shielding on dust grains, it is not immediately obvious that these trapped ion states cause a significant additional current to the dust grain. However, this effect was also found by the same researchers [5]. Even for a large ion mean free path ($\lambda_{\text{mfp}} = 10\lambda_{De}$), they found that the additional ion current due to collisions significantly affected the floating potential of the dust grain for a range of dust grain radii. This can be seen in figure 5.2, in which the addition of a collisional ion current term to the dust grain charging calculation (on top of the OML ion and electron currents) caused the potential on the grain to decrease by up to 30%. 
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This occurs because the thermal energy of ionised neutrals is so low compared to the dust grain potential \( k_B T_n \ll e\phi_d \sim k_B T_e \) that there is a large collection region surrounding the dust grain in which charge-exchange collisions will tend to create an ion with negative total energy (i.e. its negative potential energy in the grain’s potential well exceeds its kinetic energy).

Assuming an unshielded \( 1/r \) potential around a dust grain, the radius at which \( e\phi(r) = k_B T_n \) is given by:

\[
r_{\text{trap}} = \frac{e\phi_d}{k_B T_n} r_d \gg r_d.
\]  

(5.1)

Statistically, the ionisation of a neutral any closer to the dust grain is likely to produce an ion with negative total energy (a trapped ion). This leads to an effective cross section for trapped ion collection by the dust grain: \( \pi r_{\text{trap}}^2 P_{\text{coll}} \), where \( P_{\text{coll}} \) is the probability of an outside ion undergoing a charge-exchange collision while within the radius \( r_{\text{trap}} \). We can estimate the probability of a collision as \( \tau_{\text{esc}}/\lambda_{\text{mfp}} \), giving the effective collisional cross-section as:

\[
\sigma_{\text{trap}} = \pi \left( \frac{e\phi_d}{k_B T_n} r_d \right)^3 \lambda_{\text{mfp}}^{-1}.
\]  

(5.2)

For a Debye-shielded dust grain, the collection radius is estimated to extend \( \sim \lambda_D e \) from the grain, and the equivalent value is [5]:

\[
\sigma'_{\text{trap}} = \pi \lambda_D e / \lambda_{\text{mfp}}.
\]  

(5.3)

OML theory gives the collection cross-section for ions from a stationary Maxwellian distribution (the case considered by Lampe) as

\[
\sigma_{\text{i max}} = \pi r_d^2 \left( 1 + \frac{e\phi_d}{k_B T_i} \right).
\]  

(5.4)

For certain combinations of parameters, it can be seen that \( \sigma_{\text{trap}} \) may be larger than \( \sigma_{\text{i max}} \) even for a large \( \lambda_{\text{mfp}} \). This is important because, in the steady-state, the rate at which ions are deorbited (usually onto the dust grain by further collisions) must equal the rate at which they are produced - and many ions may be produced which do not even have sufficient energy to orbit the grain, and simply fall directly onto it.

The specific parameters crucial to this are the electron-neutral temperature ratio \( T_e/T_n \), which effectively determines the size of the ion-trapping region surrounding a
Figure 5.2: Floating potential reached on a dust grain surface ($\phi_d$) with trapped ion charging included, compared to the OML potential ($\phi_{d,OML}$) for varying dust grain radius, $r_d$. Reproduced from Lampe et al. [5] with slight adaptation: $\lambda_{\text{D}}/\lambda_{\text{mb}} = 0.1$. $\phi_d$ is measured relative to the distant plasma outside the trapped ion cloud.

dust grain, and the ratio between grain size and ion collision length, $r_d/\lambda_{\text{mb}}$, which determines the fraction of background ions experiencing a collision within the trapping region - and consequently the relative importance of the additional trapped-ion current to the dust grain. When an ion flow is present, the increase in ion trapping relative to the stationary case will depend on $n_i/\sqrt{T_n}$, since the ions are assumed to move at the neutral-thermal speed in this case.

It should be noted that, as in previous chapters, the collision of ions with the grain is not considered (by Lampe or in this work) to affect the mass of the grain - only its charge.

As they noted [89, 4], the model of Lampe et al. does not apply in a flowing plasma. This is largely because the inherent anisotropy surrounding a dust grain in a flowing plasma breaks the symmetries used in their analytic model and makes the scenario significantly harder to treat.
5.1.1 Flooding Plasma

The flowing plasma regime is achieved here via a computational approach, simulating a cold ion fluid moving in the potential distribution around the dust grain. Using this, we can determine the flux of ions at any point in the vicinity of the grain and thereby the rate at which charge-exchange collisions occur. We numerically simulate the trajectories of neutrals ionised by charge-exchange collisions, allowing calculation of the additional current they provide to the dust grain.

This regime is of particular interest since dust grains are commonly found in the plasma boundary, often levitated near the sheath edge. In addition, the ion flux past the dust grains in this region is greatly increased compared to in the stationary plasma treated by Lampe, and thus the collision rate near the grain is expected to increase correspondingly.

Unlike other factors which affect the charge-exchange collision rate, such as background neutral density or the collision cross-section of the ion species, a greater ion flow past the dust grain only increases the rate at which trapped-ions are created and does not affect the rate at which those ions are de-orbited by later collisions. This suggests that the ion flow increases the steady-state population of trapped ions above what Lampe et al. found, and increases the trapped-ion contribution to shielding the charge on the grain.

In turn, this higher population of trapped ions is expected to increase the trapped-ion current to the dust grain, altering its charge by a greater amount than seen in figure 5.2. As the charge on the grain, and its shielding-length are both crucial to the interaction between dust and plasma, this has the potential to fundamentally alter the dust-plasma interaction in the plasma boundary.

We consider a plasma flowing at the Bohm speed, $v_B$, with density $n_o$ and no external fields acting in the vicinity of the grain. This corresponds to a dust grain positioned at the sheath/presheath boundary, as shown in figure 5.3. The dust grain is initially charged to the steady-state OML potential, using the OML current expressions derived in Chapter 2.

The various component parts of the computational model used in this work are now introduced:
Figure 5.3: Diagram of flowing plasma scenario considered in this chapter. Ions flow at speed $v_B$ past a grain positioned at the sheath/presheath boundary. A charged dust grain (not to scale) is positioned at the sheath edge.

- a cold ion fluid model to calculate the density and flow of background ions around the dust grain
- a Jacobi relaxation method to calculate the 2D potential surrounding the dust grain
- The charge-exchange collision rate calculation, which models the rate at which trapped ions are created in the simulation domain
- A numerical integration routine to integrate the trajectory of the cold ion fluid elements and individual trapped ions

These are then combined in section 5.5 to describe the overall computational method used.

### 5.2 Cold Ion Fluid Model

In this work, the flowing plasma scenario is treated using an iterative computational approach to solve the collisionless ion fluid equations of motion self-consistently with Poisson’s equation.
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We begin by defining a spherical coordinate system \((r, \theta)\) centred on the dust grain, with the polar \(\theta = 0\) axis aligned opposite to the ion flow (pointing along the positive x-axis as defined in earlier chapters). Symmetry in the poloidal direction is assumed. This coordinate system is shown in figure 5.4. The simulation domain chosen extends from the surface of the dust grain \((r = r_d)\) to \(r = 50r_d\) and \(\theta = 0 \rightarrow \pi\).

The equation of motion for an ion fluid is given by:

\[
n_i m_i \frac{dv_i}{dt} = -\nabla P_i + n_i eE. \tag{5.5}
\]

For a cold ion fluid, \(\nabla P_i \rightarrow 0\) and the fluid parcels follow the same trajectories as individual ions. We initiate a series of ion fluid parcels at the edge of the simulation domain, \(r_o = 50r_d\) and with \(\theta_o\) distributed from \(0 \rightarrow \pi/2\), with velocity \(v = -v_B \hat{x}\). The motion of these fluid parcels is numerically integrated for a time \(dt = 100r_d/v_B\) (long enough to ensure the fluid parcels traverse the entire simulation domain) under the electrostatic force \(eE(r, \theta) = -e\nabla \phi\).

Each fluid parcel represents a number of ions \(N_i = n_o v_B 2\pi b db dt\), where \(b = r_o \sin(\theta_o)\) is the impact parameter of the fluid parcel as it enters the simulation domain and \(db\) is the difference in impact parameters between adjacent fluid elements. Dividing the simulation domain into segments of size \((dr, d\theta)\), as shown in figure 5.5, the ion density in each segment is given by:

\[
n_{l,m} = \frac{N_i \delta t_{l,m}}{2\pi r^2 \sin(\theta_m) dr d\theta dt} \tag{5.6}
\]

where \(\delta t_{l,m}\) is the time the ion fluid parcel spends in particular segment defined by \(l\) and \(m\) - the indices of the segment in \(r\) and \(\theta\), respectively \((r_l = r_d + ldr\) and \(\theta_m = m d\theta\)). The number of gridpoints in \(r\) and \(\theta\) are \(N_r\) and \(N_\theta\) respectively (such that \(l = 0, 1, 2...N_r - 1\) and \(m = 0, 1, 2...N_\theta - 1\)).

5.2.1 Angular Momentum

While a truly ‘cold’ ion fluid element will not have any motion in the poloidal direction, this leads to an unphysical situation - a singularity in the ion density behind the dust
The azimuthal coordinate $\psi$ is not widely used, since poloidal symmetry is assumed in this 2D model.

Figure 5.5: Diagram of simulation grid in $r, \theta$ with ion fluid element trajectories superimposed. Ion fluid parcels approach from the right-hand side of the simulation domain and are deflected towards the grain under the force $eE(r, \theta)$. 
grain along the $\theta = \pi$ axis. This occurs because all ions approaching the dust grain with no poloidal velocity, $v_\phi$, will cross the $\theta = \pi$ axis behind the grain.

This effect was, in fact, seen earlier in the ion trajectories shown in figure 2.5, though it was not commented on at the time since the ion density behind the grain was not relevant to the calculation being carried out.

To avoid this, the ion fluid parcels are given a small amount of initial angular momentum $L_\phi = 0.1 m_i b \sqrt{\frac{k_b T_\text{n}}{m_i}}$ to prevent them reaching the axis and causing this singularity. Since the fluid elements are shaped as rings around the azimuthal axis, this corresponds to a slightly rotating fluid element. In this manner, the fluid parcels correspond not to cold ions quite so much as very cool ions - their angular momentum corresponds to a thermal speed $\sqrt{0.01 k_b T_\text{n}/m_i}$, and with $T_\text{n} = 300 \text{K} \ll T_e$ this equates to an ion temperature $T_i = 3 \text{K}$. Thus, the ion motion is still very cold.

This angular momentum was added to the ion motion entirely for computational reasons - while some analytic theories may be able to cope with a density singularity along a line, a numerical method in spherical coordinates is less capable of dealing with such a feature. The trajectories of individual fluid elements were tracked, and this small angular momentum does not significantly affect their motion except for preventing them from passing directly through the $\theta = \pi$ axis behind the grain; the fluid parcels still pass very close to the axis, and through the computational grid-cell adjacent to the axis.

This issue could also be (perhaps better) alleviated via the use of cartesian coordinates, as long as the spherical symmetry of the simulation boundaries (particularly the inner grain-surface boundary) was carefully maintained.

### 5.2.2 Integration Method

The ion fluid parcels were integrated using a variable-order Adams-Moulton method, from the Fortran LSODA library developed at Lawrence Livermore National Laboratory [90].

The Adams-Moulton method is shown here for a function $y = f(y,t)$. It is a multistep method, whereby an initial step is made with a simple algorithm:

$$y_{n+1} = y_n + h f(y_{n+1}, t_{n+1})$$  \hspace{1cm} (5.7)

where $h = t_{n+1} - t_n$ is the step size. Later steps then make use of the information
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contained in the previous steps to apply progressively higher order methods:

\[ y_{n+2} = y_{n+1} + \frac{h}{2} \left( f \left( y_{n+2}, t_{n+2} \right) + f \left( y_{n+1}, t_{n+1} \right) \right) \]

\[ y_{n+3} = y_{n+2} + \frac{h}{12} \left( 5f \left( y_{n+3}, t_{n+3} \right) + 8f \left( y_{n+2}, t_{n+2} \right) - f \left( y_{n+1}, t_{n+1} \right) \right). \]

The LSODA library is programmed with up to a 12th order Adams integration algorithm (the formula for which is far too long to reproduce here). As can be seen, this is an implicit method, where \( y_{n+1} \) is calculated in equation 5.7 using \( f \left( y_{n+1}, t_{n+1} \right) \) (which must be solved numerically, as \( y_{n+1} \) is, of course not known at that point). Implicit methods provide great stability in numerical integration.

This numerical integration approach was chosen over a simple Runge-Kutta integration (as used earlier) due to the numerical efficiency and ease-of-use of this library, as well as the stability offered by an implicit method for longer timesteps. When low-energy trapped ions are included in this calculation (later in the chapter), this feature is particularly valuable, since particles moving at very different speeds and under different forces (closer and further from the grain) must be simulated over the same timescale without introducing inaccuracies. The library also allows a relative error threshold to be set for the quantity to be calculated (\( \sim 10^{-8} \) by default) and adjusts the order of calculation used to ensure the error stays below this value while minimising computational time.

5.3 Jacobi Relaxation

The potential surrounding the dust grain is calculated in spherical \((r, \theta)\) coordinates. Poloidal symmetry is assumed. In this coordinate system, Poisson’s equation takes the form:

\[ \nabla^2 \phi = \frac{\partial^2 \phi}{\partial r^2} + \frac{2}{r} \frac{\partial \phi}{\partial r} + \frac{1}{r^2} \left( \cot(\theta) \frac{\partial \phi}{\partial \theta} + \frac{\partial^2 \phi}{\partial \theta^2} \right) = -\frac{e}{\epsilon_o} \left( n_i - n_e \right). \]  

A Jacobi relaxation method [91] was used to calculate the potential distribution around the dust grain. In this method, Poisson’s equation is discretised \((r, \theta)\) (onto the grid described above). In this form, Poisson’s equation becomes:
The equation for the potential around the dust grain, \( \phi(0)(r, \theta) \), the Jacobi method solves the equation above for a new approximation \( \phi^{(1)}(r, \theta) \) (carrying out this update for all the points on the lattice). This operation is iteratively applied until the potential profiles converge:

\[
\phi^{(j+1)}_{l,m} = g \left[ \phi^{(j)}_{l+1,m}, \phi^{(j)}_{l-1,m}, \phi^{(j)}_{l,m+1}, \phi^{(j)}_{l,m-1} \right] + h \left[ n_{i,l,m} - n_{e,l,m} \left( \phi^{(j)}_{l,m} \right) \right].
\] (5.14)

A simple convergence criterion was applied, such that the Jacobi iteration was repeated until the change in potential in step \( j \) satisfies
\[
\max \left| \phi_{l,m}^{(j+1)} - \phi_{l,m}^{(j)} \right| < 0.01 \max \left| \phi_{l,m}^{(1)} - \phi_{l,m}^{(0)} \right| \quad (5.15)
\]
i.e. until, with each iteration, the potential is changing at less than 1% of the rate at which it initially changed with each iteration.

### 5.3.1 Ion and Electron Densities

The ion densities, \( n_{i,l,m} \), used in the Jacobi iteration are calculated from the cold ion fluid approach described above before the Jacobi iteration is begun. The electrons are modelled as Boltzmann distributed (equation 2.11).

The use of a Boltzmann distribution is justified in order to compare results from the flowing plasma model in this work with the results from Lampe et al.’s model of the stationary plasma. Such a direct comparison would not be meaningful if a different electron distribution were used. In addition, the dust grain is effectively being modelled as located at the sheath edge, where the effects of electron loss to the wall are minimal, as shown in Chapter 4.

Thus, the factors discussed in earlier chapters relating to the cutoff electron distribution need not be considered here.

### 5.3.2 Boundary Conditions

The Jacobi method requires externally fixed boundary conditions in order to perform its iteration. The first of these is chosen as an equipotential surface at the dust grain:

\[
\phi_{0,m} = \phi_d. \quad (5.16)
\]

Since the \( \theta = 0 \) and \( \theta = \pi \) boundaries are an axis of rotational symmetry, we apply the condition that there is no electric field in the \( \hat{\theta} \) direction (\( E_{\theta} \hat{\theta} = 0 \)) at these points. We do this by creating additional ‘ghost’ gridpoints just outside the boundaries and applying the condition:

\[
\phi_{r,-1} = \phi_{r,1} \quad (5.17)
\]

\[
\phi_{r,N_\theta+1} = \phi_{r,N_\theta-1}. \quad (5.18)
\]
This approach allows the radial potential variation along these axes to still be calculated. Lastly, we apply a equipotential value at the radial outer edge of the simulation, corresponding to a shielded Debye potential:

$$\phi_{N,-1,m} = \frac{c \phi_d}{r} \exp \left( -\frac{r}{\lambda_D} \right)$$  \hspace{1cm} (5.19)

where $c = (Q_d - Q_i)/Q_d$ is a factor to reduce the potential at the boundary in proportion to the trapped ion population orbiting the grain.

### 5.3.3 Weighted Jacobi Method

A slight variation on the Jacobi method was in fact used, called a weighted Jacobi method. If the Jacobi method updates the potential value by a value

$$\Delta \phi_{l,m}^{(j+1)} = \phi_{l,m}^{(j+1)} - \phi_{l,m}^{(j)}$$  \hspace{1cm} (5.20)

the weighted Jacobi method applies a smaller update:

$$\phi_{l,m}^{(j+1)} = \phi_{l,m}^{(j)} + \Omega \Delta \phi_{l,m}^{(j+1)}.$$  \hspace{1cm} (5.21)

This slows convergence slightly, but helps to prevent spurious oscillations forming in the final solution. A value $\Omega = 2/3$ was used in this work.

### 5.4 Charge-Exchange Collisions

The rate at which charge-exchange collisions ionise neutrals with a particular velocity $v_n$ (i.e. the rate of change of the trapped-ion distribution function) is given by [67]:

$$\frac{\partial f_{\text{imp}} (v_n)}{\partial t} = \iiint d^3v_i' \sigma_{ex} (v_i' - v_n) f_i (v_i') f_n (v_n) |v_i' - v_n|$$  \hspace{1cm} (5.22)

where $\sigma_{ex}$ is the ion charge-exchange cross section, and $f_{\text{imp}}$, $f_n$ and $f_i$ are the velocity distribution functions for trapped ions, neutrals, and background ions respectively. For ions moving with a speed $v_B = \sqrt{k_B T_i/m_i}$, far greater than the ion thermal speed ($\sqrt{k_B T_n/m_n}$, as used by Lampe) the ion distribution function is well approximated by a delta function $f_i (v_i) = n_i \delta (v_i)$ and the collision integral becomes:

$$\frac{\partial f_{\text{imp}} (v_n)}{\partial t} = n_i \sigma_{ex} (v_i - v_n) |v_i - v_n| f_{\text{max}} (v_n).$$  \hspace{1cm} (5.23)
The neutral velocity distribution function is assumed to be Maxwell-Boltzmann:

\[
    f_n(v_n) = f_{\text{max}}(v_n) = n_{\text{neut}} \left( \frac{m_i}{2 \pi k_B T_n} \right)^{3/2} \exp \left( \frac{-m_i v_n^2}{2 k_B T_n} \right).
\]  

(5.24)

Since the ion speed is far greater than the neutral thermal speed, this collision integral approximates further to:

\[
    \frac{\partial f_{\text{trap}}(v_n)}{\partial t} = n_i \sigma_{\text{ex}}(v_i) |v_i| f_{\text{max}}(v_n).
\]  

(5.25)

The total rate of ionisation by charge-exchange collisions in a volume \(dV\) is then

\[
    \frac{\partial N_{\text{trap}}}{\partial t} = n_{\text{neut}} n_i \sigma_{\text{ex}}(v_i) |v_i| dV.
\]  

(5.26)

The charge-exchange cross section for Argon is measured experimentally in reference [92] for a range of ion energies, giving the result:

\[
    \sigma_{\text{ex}}(E_{ev}) = \left( 7.49 \times 10^{-10} + 0.73 \times 10^{-10} \ln E_{ev} \right)^2 \text{m}^2
\]  

(5.27)

where \(E_{ev}\) is the ion energy in electron volts. Another similar measurement (with comparable values) can be found in [93], and could be used in place of this. Since the parameter combination \(n_{\text{neut}} \sigma_{\text{ex}}\) controls the collision rate, and \(n_{\text{neut}}\) can take a wide range of values, the choice of which of these numerical values to use for \(\sigma_{\text{ex}}\) is not crucial to the results below.

### 5.5 Computational Approach

Initially, an unshielded, symmetric potential \(\phi(r) = \phi_d r_d\) is imposed, and a set of cold ion fluid trajectories integrated under this potential. This allows \(n_i(r, \theta)\) to be calculated using equation 5.6. 3000 ion fluid parcels were used to obtain a high resolution for the density around the dust grain.

This allows Poisson’s equation to be evaluated, using the Jacobi relaxation method detailed in section 5.3, to give an updated potential profile. This process is iterated until the ion density and potential profiles converge.

Once the cold ion fluid and Jacobi relaxation methods have calculated a set of self-consistent ion density and electrostatic potential distributions around the dust grain,
the time-evolution of the simulation is begun. The following sequence of calculations are done repetitively:

1) The charge-exchange collision integral is evaluated in every computational segment \((dr, d\theta)\) to calculate the number of trapped ions produced in a time \(\Delta t\):

\[
\delta N_{l,m} = \frac{\partial N^+}{\partial t}(r_l, \theta_m) \Delta t.
\]

\(\delta N_{l,m}\) is calculated for each computational cell, and this number of trapped ions is added to the simulation domain with velocities drawn randomly from \(f_{\text{max}}(\xi_n)\).

Ions produced with total energy \(E_{\text{tot}} = \frac{1}{2}m_i v_i^2 + e\phi(r, \theta) > 0\) are ignored and not calculated, since these only leave the simulation (sometimes very slowly) taking up computational time while not contributing to charging or long-term shielding of the grain.

2) We numerically integrate the motion of the trapped ions (under the same equation of motion and using the same integration method as the cold ion fluid parcels above) for a timestep \(\Delta t\) to discover whether they follow orbital trajectories, escape the grain, or collide with it.

3) The charge on the grain is then updated by a value:

\[
\Delta Q = (I_e + I_i) \Delta t + \Delta Q_{\text{trap}}
\]

where \(I_e\) and \(I_i\) are the electron and ion currents from OML theory and \(\Delta Q_{\text{trap}}\) is the number of trapped ions whose trajectories collided with the dust grain in time \(\Delta t\).

4) The Jacobi relaxation method is used to calculate an updated potential distribution around the grain, including the trapped ion contribution in the ion number density \(n_i\).

5) The cold-ion fluid code then recalculate the background (untrapped) ion density. This effectively assumes that the background plasma equilibrates instantly as trapped ions are generated.

6) In addition, during each timestep, there is a probability \(dP\) of a trapped ion
undergoing a further charge-exchange collision. This is calculated, using the same approximations as above:

\[ dP = n_{\text{neut}} \sigma_{\text{ex}} (v) \, |v| \Delta t. \quad (5.30) \]

A Binomial random number generator decides, for each ion, whether a collision occurs. If so, the computational ion is replaced at the same location by an ion with velocity randomly sampled from \( f_{\text{max}} \). This allows the possibility of orbiting ions being deorbited by further collisions, rather than trapped indefinitely.

These stages are repeated iteratively until the chosen number of timesteps have been completed. The number of timesteps was chosen manually in order to ensure sufficient time elapsed in the simulation for the trapped ion charge to evolve, and the charge on the grain to decrease to its new steady state value (this being determined by inspection).

An automated end criterion could also be implemented, to be chosen depending on the physical processes of interest.

5.6 Numerical Testing

Various numerical tests were used to ensure the reliability of results from this model. The Jacobi relaxation scheme was tested in analytically verifiable scenarios, such as a the limit of \( r_d/\lambda_{\text{De}} \to 0 \), in which case the scheme relaxes to \( 1/r \) potential around an unshielded sphere, even for arbitrary initial forms for the potential. This is shown in figure 5.6, where an initially parabolic potential profile can be seen progressively relaxing to the correct potential form.

The Jacobi algorithm was also tested for finite \( r_d/\lambda_{\text{De}} \), with \( n_e \) retaining its Boltzmann distribution but \( n_i \) set to a constant background density. In this case, the analytic solution - a Debye shielded potential - was again recovered; this is shown in figure 5.7.

Other tests included setting the charge-exchange cross section to zero (i.e. removing trapped ions from the simulation), and calculating the background ion current to the
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Figure 5.6: Potential distribution surrounding an unshielded dust grain, iterating to converge to analytic solution $\phi_a$.
$\phi_0$ represents the ‘guessed’ potential distribution, which is applied as the starting point for the Jacobi scheme; $\phi_1$, $\phi_2$, and $\phi_3$ represent progressively later stages in the iteration, and progressively approach the analytic solution.

Figure 5.7: Potential distribution surrounding a Debye-shielded dust grain (for $50r_d = 2\lambda_{De}$), iterating to converge to analytic solution $\phi_a$.
$\phi_0$ represents the ‘guessed’ potential distribution, which is applied as the starting point for the Jacobi scheme; $\phi_1$, $\phi_2$, and $\phi_3$ represent progressively later stages in the iteration, and progressively approach the analytic solution.
CHAPTER 5. TRAPPED ION THEORY

grain from the fluid code. The ion current which was found to match the OML value, and the grain remained at the OML potential without deviation in this scenario.

The code to move ions within the simulation domain was also tested using energy conservation as a measure of accuracy. This was done first for individual ions, in which case the ion energy remained constant throughout the integration, and then for an ensemble of ions moving together within the grain’s potential well.

This was done by setting the grain charge to a constant value and introducing a population of trapped ions within the simulation domain; the code was run with the shape of the potential allowed to vary between steps (as usual), but with no additional trapped ions created beyond the initial population and the grain charge also not allowed to evolve with time. These features exist in the simulations detailed in the next chapter, but were disabled for this test since allowing the charge within the simulation domain to change inherently changes the total energy of the system - rendering the energy conservation test invalid.

As can be seen in figure 5.8, which shows the fractional ion energy change over a number of simulation steps, the energy of most ions remains relatively constant (to within $< 2\%$). The energy variation still present is caused by the fact that over the simulation steps, some of the trapped ions leave the simulation domain and the total charge in the situation therefore changes. This is not an inherently unphysical energy change, however, and cannot easily be removed from the simulation to enable even more thorough testing.

The few ions whose energies vary by more than $\sim 2\%$ represent ions with a very small total energy (since ions are generated from a Maxwellian distribution); since the figure is scaled by the initial ion energy $E_o$ any change appears large for these few ions.
Figure 5.8: Fractional energy change of ~ 80 trapped ions in a dust grain potential well. \( E_i \) represents the total energy (kinetic and potential) of ions with initial energy \( E_0 \), changing (or remaining constant) between steps in the simulation.
Chapter 6

Trapped Ion Results

In this Chapter, results from the model described in the previous Chapter are presented and their implications discussed.

The simulation was initiated with the dust grain charged to the steady state OML potential at the sheath edge ($\tilde{\phi}_d = 3.81$, which corresponds to a charge $Q_d \approx 27,000e$). The simulation was then run for 250 timesteps $\Delta t$, in the manner described above, with the timestep adaptively changing to limit the production of trapped ions in each step to no more than $0.02Q_d$. This ensures that the potential distribution around the grain does not change excessively with each timestep. The computational grid in $(r, \theta)$ was initiated with 100 radial intervals $dr$, and 30 azimuthal intervals $d\theta$.

The dust grain parameters were chosen to correspond closely to Lampe’s, to allow direct comparison: $r_d = 5\mu m$ and $\lambda_{De} = 332\mu m$ (such that $r_d/\lambda_{De} = 0.015$), and background neutral gas at $T_n = 300K$ with density $n_{neut} = 5.0 \times 10^{20} m^{-3}$, with plasma density $n_o = 10^{15} m^{-3}$ and electron temperature $T_e = 2eV$ such that $T_n/T_e = 0.013$). This gives a mean free path $\lambda_{mfp} = 10\lambda_{De}$, far greater than the $50r_d$ simulation domain.

This also ensures that the simulation domain, radius $50r_d$, $\approx 0.75\lambda_{De}$ - much smaller than the sheath scale.

6.1 Grain Charging

The evolution of charge on the dust grain and in the surrounding cloud of trapped ions is shown in figure 6.1. The final (steady-state) charge on the dust grain was found to be $Q_d = 12,800e$, or $\sim 45\%$ of the initial (OML-calculated) charge on the grain. For
reference on the timescales involved, $1000 v_d / v_H = 2.3 \mu s$ for a 5$\mu m$ dust grain.

This is a far greater effect than seen in the stationary case, where the floating potential on the dust grain never decreased more than 30%. The difference is due to the large trapped-ion current to the grain, as shown below in figure 6.2. The trapped-ion current can be seen to greatly exceed the standard ion current to the grain, due to the increased rate at which charge-exchange collisions produce trapped ions under these conditions.

It can also be seen that, as the grain potential becomes less negative, the electron current increases to compensate – and the new steady state is reached when the electron current equals the increased ion current.

As the charge on the dust grain ($Q_d$) decreases and the charge in the surrounding trapped ion cloud ($Q_{\text{trap}}$) increases, the potential well surrounding the grain shrinks and the rate of trapped ion production decreases. As a result, the trapped-ion current to the dust grain decreases. However, this response is not instantaneous – there is a delay as existing trapped ions find their way to the dust grain (or out of the simulation domain, since the decreased dust grain potential may be insufficient to keep ions trapped).

This results in the oscillation in $Q_{\text{trap}}$ and $Q_d$ seen in figure 6.1, and later in figure 6.3.
Figure 6.2: Time evolution of current to the dust grain from trapped ions, electrons, and untrapped ions.

6.2 Grain Shielding

The charges shown in figure 6.1 are shown as a ratio in figure 6.3. The final charge in the trapped ion cloud is $\sim 66\%$ of the charge on the dust grain, almost 50\% greater than in the stationary case considered previously by Lampe et al.

Figure 6.4 corresponds to Lampe’s figure 5.1 in the previous chapter, showing the separate sources of space-charge once the steady-state is reached. This is done in one-dimension here, integrating over $\theta$.

Unlike in the Lampe case, where the grain potential was still shielded over several $\lambda_{De}$, the shielding scale here is significantly smaller ($50r_d \approx 0.75\lambda_{De}$) and the shielding is very much dominated by the trapped ion space-charge.

The scale over which shielding occurs is a consequence of the rate of production of trapped ions. The generation of trapped ions by collisions increases the shielding of the potential around the grain, effectively decreasing the size of the potential well; however a smaller potential well offers a decreased volume within which ion-trapping
collisions can occur, and decreases the rate of trapped ion generation. This negative feedback mechanism causes the grain-shielding radius to reach steady state at a value where trapped ion generation matches the rate at which these ions are lost to the grain. In the flowing case, far more trapped ions are generated per unit volume in the vicinity of the grain (due to the high ion flux), so this steady-state radius is much smaller than in the case considered by Lampe.

The 2D potential distribution around the grain is shown in figure 6.5. The radial potential variation along the $\theta = 0$ axis (directly upstream of the grain) is then shown in figure 6.6. In the latter figure, a potential curve corresponding to $Q_{\text{trap}} = 0$ is also shown, to compare the shielding scale-lengths with and without trapped ions. The potential can be seen to fall significantly faster with trapped ion shielding included.

Also shown is a $1/r^2$ potential distribution, showing that even with the grain potential shielded over this significantly reduced scale, the potential still does not vary as steeply as $1/r^2$. This is significant because it shows that one aspect of the OML theory still holds in this regime - the potential does not vary steeply enough for for absorption barriers to affect the collection of ions by the dust grain, as discussed in Chapters 1 and 2.
CHAPTER 6. TRAPPED ION RESULTS

Figure 6.4: Total space-charge within a radius $r$ of the dust grain. $Q_{\text{trap}}$ is total trapped ion charge within a radius $r$. $Q_t + Q_e$ are the sum of (untrapped) ion and electron space-charge, corresponding to normal Debye shielding.

Figure 6.5: The potential distribution surrounding the dust grain. The positive x-direction corresponds to $\theta = 0$ (i.e. towards the incoming ion flow).
Figure 6.6: Potential distribution surrounding the dust grain along $\theta = 0$ axis.
6.3 Ion Wake

As mentioned earlier, dust grains have a tendency to focus the ion flow downstream of the grain. This produces an effect known as an ion wake [94], which persists some distance downstream of the grain. For small grains, this wake is of interest in the formation of plasma crystals, as dust in the wake of an upstream grain tends to be held in this wake by a force if the upstream grain is moved [95].

This wake effect is also altered, as a result of the trapped ions. The wake behind the dust grain at the beginning and end of the simulation are both shown, in figures 6.7 and 6.8 respectively, with a significantly (over 20%) lower density seen in the wake after trapped ion charging and shielding are accounted for.

The singularity avoidance strategy (detailed in section 5.2.1) should not have impacted these results, since the ion fluid elements were able to pass well within the final computational grid cell adjacent to the $\theta = \pi$ axis, just not directly through the axis. It should be noted, though, that for a plasma with larger finite ion temperature $\approx T_n$, the wake may look significantly different to a cold-ion-model wake due to the finite thermal motion (and therefore significant angular momentum) of the ions.

This is only an example of the many ways the different scale and shape of the sheath potential caused by trapped ions can affect the dust-plasma interaction.
Figure 6.7: Wake behind the dust grain under simulation initial conditions, with no trapped ion shielding.

Figure 6.8: Wake behind the dust grain under simulation final conditions, with trapped ion shielding.
CHAPTER 6. TRAPPED ION RESULTS

6.4 Smaller Dust Grain

An additional simulation carried out at a smaller dust grain radius, \( r_d = 1 \mu m \) (and with all other plasma parameters the same), produced an interesting result. As in the 5\( \mu m \) case, the the trapped ion shielding charge evolved to around two-thirds of the charge on the grain, as shown in figure 6.9. The trapped ion current was also found to again be dominant over the background ion current (figure 6.10).

Intuitively, one might expect the trapped ion current to be less significant at this smaller scale since the rate of trapped ion generation will have decreased by a factor of \( r^3 \) (in this case 125) compared to the 5\( \mu m \) grain above, while the OML background
currents only have an $r^2$ dependence on grain radius (see chapters 2 and 5 for discussion of these scalings), and would thus have decreased less.

Interestingly, however, the trapped ion current was found to be even more significant (and more dominant over the background ion current) than in the 5μm case above. This can be seen in figure 6.11, where the charge on the grain drops to $\sim 30\%$ of its initial (OML) value due to the added trapped ion current, while the 5μm reached steady state at $\sim 45\%$ of the OML value (and never went below 40%).

This is believed to occur because not all trapped ions will be in orbit; the term includes any ion with insufficient energy to escape the grain potential well. Many of these, particularly those generated by collisions closer to the grain may also have insufficient energy to orbit the grain. Thus, these ions fall directly onto the grain, only contributing to the shielding during their fall.

For a smaller dust grain, this turnover will be faster, since the physical distance between trapped ion generation (via a collision) and the grain surface is reduced. As such, the smaller grain can have a similar level of shielding from trapped ions, while maintaining a high trapped ion current to the grain.
Figure 6.11: Total charge on the grain and in the trapped ion cloud (for 1μm grain), evolving over time from the initial QML charge.

The lifetime of trapped ions for this grain size is shown in figure 6.12, where it can be seen that trapped ions typically collide with the dust grain (and a relatively few exit the simulation via the outer boundary, due to de-trapping by the shrinking grain potential), within a significantly shorter time than the grain charging timescale. In the steady-state, this lifetime also represents the timescale for trapped ion creation.

Consequently, the scaling of this effect with grain size may be more complex than initially intuited, and additional work for a range of grain sizes would be of interest to discern the scaling behaviour.

6.5 Discussion
In Chapter 4, it was seen that a change in dust grain charge causes the force-balance on the grain to differ greatly, with significant consequences for dust grain dynamics in the sheath. A > 50% reduction in charge on the grain, such as seen here, will greatly decrease the energy required for a dust grain to overcome the sheath potential barrier and collide with the wall. In addition, it will reduce the energy imparted to dust grains
which are ejected from the wall by sputtering or other erosion processes. Both of these are of interest for considering dust contamination of plasmas, and certainly for any of the plasma processes (discussed in Chapter 1) in which dust is intentionally introduced into the plasma for various purposes.

As well as altering the force-balance on the grain, the shielding provided by trapped ions fundamentally changes the scale over which small \( r_d < \lambda_{De} \) dust grains interact with the plasma. This was seen in the ion wake results above, but has additional consequences for other dust-plasma interactions such as the ion-drag force, which would be expected to decrease significantly as a consequence. The interaction between dust-grains, which create states such as the dust-plasma crystal [96] seen in figure 1.3 would also be expected to change, though the consequences here are less clear.

The shielding provided by these trapped ion states differs significantly from standard Debye shielding in that trapped ions are incapable of leaving the grain’s potential well. As such, the grain and orbiting ions may act as effectively a single charge under the effect of an externally imposed electrostatic field - in a similar way to the manner in which atoms or ions move as a single charged (or uncharged) object under an electric field despite being composed of many charged particles.
The possibility of this behaviour is very significant because if they do undergo motion as a single object, the grain and trapped-ion cloud described in this Chapter would have a combined charge of just $\sim 15\%$ that of the original OML-predicted charge on the grain.

Investigating this phenomenon further, it is also very possible that a regime will be found in which almost the entire charge on the dust grain will be shielded by trapped ions. In this case, the grain and charge cloud may act as a ‘dust atom’ - a much larger analogue to a classical atom.

Depending on the level of sensitivity this increased trapping has to the ion flow-speed, this effect may also extend far beyond the sheath, and well into the presheath. In addition, the progressively faster ion flow deeper into the sheath may increase this effect even further. However, this will be limited by the sheath electrostatic field which, at sufficiently high values, may pull otherwise trapped ions out of the grain’s potential well. This would be equivalent to ‘ionising’ the dust atom structures discussed in the previous paragraph.
Chapter 7

Conclusions and Discussion

This thesis documents research on the charging of individual small dust grains ($r_d < \lambda_{De}$) in the edge region of a plasma. Chapter 1 explained the context of the plasma boundary and its importance to various plasma applications. The basic physics of the plasma sheath was explained, and the common phenomenon of dust-contamination of plasmas was introduced.

Two separate effects were identified as having possible impact on modelling dust in the plasma boundary, one relating to electron dynamics in the sheath, the other relating to ion motion.

7.1 Non-Boltzmann Electrons

A fluid model for the collisionless, cold-ion sheath in an RF-driven plasma was derived in Chapter 2, along with the Orbital Motion Limited theory of dust grain charging. This model, which uses Boltzmann-distributed electrons, represents a common approach to the modelling of the plasma boundary.

Since the Boltzmann electron model ignores electron absorption by the sheath wall, a simple upgrade to this model was described in Chapter 3 to address the issue by removing electrons absorbed by the wall from the Maxwell-Boltzmann velocity distribution (since these are unphysical). This conceptually simple change has mathematically complex consequences for modelling the sheath. The sheath electron density and flux to the wall were re-derived, for both the simple case of a monotonic sheath potential and the more challenging case of a sheath with an electric field-reversal.

The electron current to a dust grain was also derived for this new velocity distribu-
tion, for each of the various charging conditions discussed in Chapter 3.

In Chapter 4, the results of the two models (referred to as CC - cutoff correction - and BE - Boltzmann electron - respectively) were compared. The potential profiles at the peak of the sheath oscillation were found to be markedly different, with the CC model predicting later onset of the field-reversal and a smaller potential on the wall for high RF driving voltages.

The impact on dust charging was then investigated, with the dust grain potential profiles progressively departing from those predicted by the BE model. This then has an impact on the forces experienced by dust grains and their motion in the sheath. This is particularly shown in figures 4.11 and 4.12, in which dust grains launched from the wall require far more initial energy in the CC model in order to avoid returning to hit the wall, but are able to reach the wall with far lower initial energies if launched from the sheath edge.

This has potential consequences for dust contamination of plasma-processing surfaces, as dust colliding with a plasma processing surface has the potential to cause damage to the surface. If this model can be extended to higher temperature, lower ion mass plasmas, it may also have consequences for dust in the edge of a tokamak. In this case, it could affect how easily dust can reach the core plasma and cause contamination there.

7.1.1 Future Work

This model provides a computationally inexpensive approach to modelling the sheath edge with increased physical accuracy compared to the BE model. Having shown the impact that electron absorption by the wall can have in the (relatively) simple case of a collisionless cold-ion sheath, this work could be extended with relative ease to other regimes.

Collisional-ion sheath profiles have been modelled by Nitter [55] and shown to increase the electron density within the sheath. The ion model used in this work could be adapted to this collisional form without changing the electron modelling, and the increased electron density makes this regime of interest to investigate.

In addition, as can be seen from equation 2.17, lower-mass ions have a higher Bohm speed and result in a smaller potential difference ($V_{dc}$) across the sheath. As a result,
it could be of interest to find out whether the CC model departs from BE at lower RF voltages (or even with $V_{rf} = 0$) for other ion species.

An extension which is of particular interest is relaxing the assumption that the sheath wall is cold and does not thermonically emit electrons, or emit them due to ion/electron impacts. In a regime where these processes occur (for example a tokamak plasma-facing component), there will be an additional electron population within the sheath near the wall. Not only should this additional electron density near the wall increase the magnitude of the field reversal directly, but the emission process will also cause the wall to gain a less negative charge - allowing more electrons from the plasma further into the sheath, and increasing the field reversal in this manner as well.

Lastly, evaluating the electron density and OML currents for a bi-Maxwellian electron velocity distribution would be a sensible extension to this model. These are a more common velocity distribution in the plasma boundary, and are the sensible next step for this investigation.

Part of the purpose of this work was to produce a (relatively) computationally inexpensive model of the sheath which does not disregard electron loss to the wall. Since the shape of the distribution in this model is not changed by kinetic effects within the sheath, an analytic modification to OML for dust grains could be derived for use with it, as well.

Use of a Vlasov code to model this more complicated sheath would, however, be of interest as it would allow investigation of collisionless electron heating processes and collisions with ions & neutrals, which both act to change the shape of the electron velocity distribution; in this manner, the parameter-space in which the fluid model is applicable could be determined.

## 7.2 Collisions

In Chapter 5, an ion fluid model to resolve the two-dimensional ion density and electrostatic potential surrounding a dust grain at the sheath edge was devised. This allowed the rate of ion collisions to be calculated and a hybrid code used to calculate the motion of trapped ions, as well as their contribution to the charging and shielding of the dust grain.

This work was an extension of previous work done to investigate the same phenomenon in a stationary plasma. Similar length-scales were used in this work, to allow
CHAPTER 7. CONCLUSIONS AND DISCUSSION

direct comparison of the two scenarios. As expected, the high ion flow past the dust grain significantly increased the number of trapped ions surrounding the dust grain compared to the stationary plasma case, with trapped ions shielding the majority of the charge on the grain. In addition, the ion current to the dust grain was greatly increased by collisions, leading to a more than 55% reduction in the steady-state charge on the grain.

Significantly, trapped ions were found to provide a mechanism for charge shielding to occur over a length-scale $< \lambda_{De}$. This has the potential to significantly change the manner in which dust grains interact with the plasma near the sheath edge.

7.2.1 Future Work

The shielding provided by these trapped ion states differs significantly from standard Debye shielding in that trapped ions are incapable of leaving the grain's potential well. As such, the grain and orbiting ions may act as effectively a single charge under the effect of an externally imposed electrostatic field.

However, the application of sufficiently large external fields (such as the field deeper within the sheath region) may also limit this effect. A sufficiently strong field will do the equivalent of ionizing these atom-like structures, and de-trap ions from the grain’s potential well. Thus, these structures would not be expected to survive deep in the sheath. This effect of an external electrostatic field is, in either case, worthy of investigation.

In addition, testing the value of the trapped-ion current for a wider range of dust grain sizes and ion flow speeds would be of interest, to find the range of parameters for which this increased ion trapping occurs. The dependence on ion speed is of particular interest, as investigating lower ion speeds would allow the model to be extended into the presheath region, while higher ion speeds are relevant deeper in the plasma sheath.

This future work is likely to be done using a Particle-In-Cell simulation approach, as this will allow the background ion motion to be better treated at lower flow speeds (where the ion thermal motion is more important). The zero-flow case could then be compared to Lampe’s results for this situation.

In addition, a Particle-In-Cell approach could treat the generation of trapped ions more simply, as a charge-exchange collision could be modelled simply via a PIC ion losing energy (and momentum) - rather than treating the trapped and background ion
populations totally distinctly.

7.3 Combining the Effects

While these two effects may seem quite somewhat separate, with one relating to ions and the other to electrons, they both provide significant changes to the manner in which small dust grains interact with an edge-plasma. Both act to decrease the dust grain charge below the OML value, as predicted in certain experiments \[22\]. The region in which the cutoff-correction fades (close to the sheath edge) is also the region in which the trapped ion effect has been shown in this work to be significant. Thus, the two effects can together cause a reduced dust grain charge across the entire edge-plasma region. Where the two overlap, the effects seen in Chapter 4 would likely be enhanced, changing the forces acting on the dust grain, and its motion in the sheath, to an even greater degree than was found in Chapter 4 of this work.

Trapped ion charging near the sheath edge may even cause grains to levitate lower in the sheath than otherwise, bringing them into the region where the cutoff acts.

Combining these effects into a larger simulation of the dust-plasma interaction in the sheath (and presheath), along with other known sheath effects not considered in this work, is planned in order to give an accurate calculation of various dust grain effects throughout the plasma-edge.

Quantities of interest may include the maximum size dust grain which can be levitated stably in a sheath, the energy imparted to a dust grain as it is ejected from the wall and where its trajectory takes it, and the nature of dust interactions with other dust grains (and their surrounding ion clouds). The initial launching of particles from a tokamak wall is of particular interest, as this could be combined into a larger simulation such as DTOKS \[97\] which predicts dust grain motion throughout a tokamak and finds where dust is deposited in the tokamak plasma (or redeposited on the wall).
Bibliography


Appendix A: Extended Derivations

Equation 1.2

We consider a plasma with two charged species, positively charged ions and negative electrons. Far from the wall, we assume quasi-neutrality (i.e. that, apart from stochastic fluctuations, the plasma has no net charge):

\[ Z n_{i0} = e n_{e0} \]

where \( n_{i0} \) and \( n_{e0} \) are, respectively, the ion and electron densities density far from the wall (in an unperturbed region of the plasma), \( e \) is the magnitude of the electronic charge, and \( Z \) is the ionisation number of the ion species.

Since electrons are the more mobile species, we assume that they respond to the potential around the charged surface far faster than the ions, and move to shield the charge on the wall while the ions remain immobile. We assume that electrons reach an equilibrium in the potential distribution around the wall, and thus apply the Boltzmann relation for their density:

\[ n_e (\phi) = n_{e0} \exp \left( \frac{e\phi}{k_B T_e} \right) \]

where \( \phi (x) \) is the potential near the wall relative to a reference potential \( \Phi = 0 \) far from the wall, \( k_B \) is Boltzmann’s constant, and \( T_e \) is the electron temperature in the plasma.

This assumption of thermal equilibrium is broken by the fact that the wall acts as a sink for incident electrons; however this is discussed at length in Chapters 3 and 4, and need not be addressed here also.

We insert this electron density into Poisson’s equation, along with the constant ion density \( n_i = n_{i0} \):
\[
\frac{\partial^2 \Phi}{\partial x^2} = -\frac{e}{\epsilon_o} (Zn_i - n_e)
\]

\[
\frac{\partial^2 \Phi}{\partial x^2} = -\frac{e}{\epsilon_o} \left( Zn_{io} - n_{eo} \exp \left( \frac{e\Phi}{k_B T_e} \right) \right) = -\frac{en_{eo}}{\epsilon_o} \left( 1 - \exp \left( \frac{e\Phi}{k_B T_e} \right) \right).
\]

An analytic solution may be found for small \( \Phi \ll k_B T_e/e \), in which case a first-order expansion of the exponential term gives:

\[
\frac{\partial^2 \Phi}{\partial x^2} = -\frac{en_{eo}}{\epsilon_o} \left( 1 - \left[ 1 + \frac{e\Phi}{k_B T_e} \right] \right)
\]

\[
\frac{\partial^2 \Phi}{\partial x^2} = -\frac{en_{eo}}{\epsilon_o} \left( 1 - \left[ 1 + \frac{e\Phi}{k_B T_e} \right] \right) = \frac{e^2 n_{eo}}{\epsilon_o k_B T_e} \Phi.
\]

This may be recognised as a harmonic solution of the form:

\[
\frac{\partial^2 \Phi}{\partial x^2} = \frac{1}{\lambda_{De}^2} \Phi
\]

where \( \lambda_{De} = \sqrt{\frac{\epsilon_o k_B T_e}{n_{eo} e^2}} \) is the electron Debye length - the length scale over which charges are typically shielded out in a plasma. The potential distribution then takes the shape:

\[
\Phi(x) = V_{wall} \exp \left( \frac{-x}{\lambda_{De}} \right)
\]

where \( V_{wall} = \Phi|_{x=0} \) is the potential at the wall, and the potential decays exponentially away from the wall over several Debye lengths. This exact form of the potential will not hold close to the wall, where the potential may be large (invalidating the first-order expansion done above). However, it illustrates the approximate form of the potential, and the scale over which charges are shielded.

**Equation 2.3**

The Bohm criterion can be derived (as done in reference [13]) beginning with the normalised Poisson’s equation, and inserting the Boltzmann relation (equation 2.11) for the electron density.

For the ion density, a variant on equation 2.6 is used, altered to have the ions entering the sheath at an unknown normalised speed \( \tilde{v}_{io} = v/v_B \), rather than the Bohm
speed (with the aim of proving that $\tilde{v}_{io} \geq 1$).

$$\frac{\partial^2 \tilde{\phi}}{\partial \tilde{x}^2} = \tilde{n}_e - \tilde{n}_i$$

$$\frac{\partial^2 \tilde{\Phi}}{\partial \tilde{x}^2} = \exp \left( \tilde{\phi} \right) - \left( 1 - 2 \frac{\tilde{\Phi}}{\tilde{v}_{io}} \right)^{-1/2}.$$
to the wall; however, the Bohm criterion can also be shown to hold without modification for RF driven discharges [98].

**Equation 2.23**

The monoenergetic ion current to a dust grain may be obtain from the OML formula as follows. We begin by combining equations 2.21 and 2.22:

\[
I_i(\phi_d) = e\pi r_d^2 \iiint v_o \left( 1 - \frac{2e\phi_d}{m_i v_o^2} \right) f_i (v_o) \, d^3v_o
\]

where \( f_i \) is the ion velocity distribution function. In the monoenergetic case, this distribution is described by a delta function, \( f_i = n_i \delta (v_i) \). Inserting this into the equation above gives an easily integrable function since, for any function \( g(x') \),

\[
\int g \left( x' \right) \delta (x) \, dx' = g (x)\text{.}
\]

Thus, the ion current becomes:

\[
I_i(\phi_d) = e\pi r_d^2 \iiint v_o \left( 1 - \frac{2e\phi_d}{m_i v_o^2} \right) n_i \delta (v_i) \, d^3v_o = e\pi r_d^2 v_i n_i \left( 1 - \frac{2e\phi_d}{m_i v_i^2} \right).
\]

By applying the ion continuity and energy conservation equations (2.4 and 2.5 respectively) and normalising the potentials, this formula can then be altered into into the form seen in equation 2.23:

\[
I_i(\phi_d) = n_o e\pi r_d^2 v_B \left( 1 + \frac{2\phi_d}{2\Phi_{dc} (x) - 1} \right).
\]

**Equations 2.24 and 2.25**

The electron current to the grain is slightly more complicated to calculate than the ion current. We begin again by combining equations 2.21 and 2.22:

\[
I_e(\phi_d) = -e\pi r_d^2 \iiint v_o \left( 1 + \frac{2e\phi_d}{m_e v_o^2} \right) f_e (v_o) \, d^3v_o.
\]

Since the electron velocity distribution is modelled as a Maxwell-Boltzmann, which is isotropic in velocity space, \( f_e \) is given by:
\[ f_e(v_o) = n_e \left( \frac{m_e}{2\pi k_B T_e} \right)^{3/2} 4\pi v_o^2 \exp \left( -\frac{m_e v_o^2}{2k_B T_e} \right) \]

which depends only on the magnitude of the electron velocity. Therefore, we can reduce the integral to a one-dimensional form:

\[ I_e(\phi_d) = -e\pi r_d^2 \int_{v_{\text{min}}}^{\infty} v_o \left( 1 + \frac{2e\phi_d}{m_e v_o^2} \right) n_e \left( \frac{m_e}{2\pi k_B T_e} \right)^{3/2} 4\pi v_o^2 \exp \left( -\frac{m_e v_o^2}{2k_B T_e} \right) dv_o \]

where \( v_{\text{min}} = \sqrt{-\frac{2e\phi_d}{m_e}} \) is the minimum approach speed for an electron to reach the dust grain (from energy conservation).

We substitute the normalised variables \( \tilde{v}_o = \frac{v_o}{\sqrt{k_B T_e/m_e}} \) and \( \tilde{\phi}_d = e\phi_d/(k_B T_e) \) into this equation to simplify it:

\[ I_e(\phi_d) = -4n_e e\pi r_d^2 \sqrt{\frac{k_B T_e}{8\pi m_e}} \int_{\tilde{v}_{\text{min}}}^{\infty} \tilde{v}_o^3 \left( 1 + \frac{2\tilde{\phi}_d}{\tilde{v}_o^2} \right) \exp \left( -\frac{\tilde{v}_o^2}{2} \right) d\tilde{v}_o \]

where \( \tilde{v}_{\text{min}} = \frac{v_{\text{min}}}{\sqrt{k_B T_e/m_e}} \). For a positively charged dust grain (\( \tilde{\phi}_d > 0 \)), electrons are attracted to the dust grain and \( \tilde{v}_{\text{min}} = 0 \); the OML current is evaluated in this regime, using the standard integrals:

\[ \int_0^{\infty} x^3 \exp \left( -\frac{x^2}{2} \right) dx = 2, \quad \int_0^{\infty} x \exp \left( -\frac{x^2}{2} \right) dx = 1. \]

This gives equation 2.25, the OML electron current to a positive dust grain:

\[ I_e(\phi_d) = -4n_e e\pi r_d^2 \sqrt{\frac{k_B T_e}{8\pi m_e}} \left( 2 + 2\tilde{\phi}_d \right) = -n_e e\pi r_d^2 \sqrt{\frac{8k_B T_e}{\pi m_e}} \left( 1 + \tilde{\phi}_d \right). \]

In the case of a negatively charged dust grain, \( \tilde{\phi}_d < 0 \), we use a different set of standard integrals since \( \tilde{v}_{\text{min}} > 0 \):

\[ \int_a^{\infty} x^3 \exp \left( -\frac{x^2}{2} \right) dx = (a^2 + 2) \exp \left( -\frac{a^2}{2} \right), \quad \int_a^{\infty} x \exp \left( -\frac{x^2}{2} \right) dx = \exp \left( -\frac{a^2}{2} \right). \]
This gives the OML current to a negatively charged dust grain (equation 2.24):

\[ I_e(\phi_d) = -4n_e e \pi r_d^2 \sqrt{\frac{k_B T_e}{8\pi m_e}} \left( \left( \tilde{v}_{\text{min}}^2 + 2 + 2\tilde{\phi}_d \right) \exp \left( -\frac{\tilde{v}_{\text{min}}^2}{2} \right) \right). \]

Since \( \tilde{v}_{\text{min}}^2 = \frac{v_{\text{min}}^2}{k_B T_e/m_e} = -2\tilde{\phi}_d \), this can be reduced to:

\[ I_e(\phi_d) = -n_e e \pi r_d^2 \sqrt{\frac{8k_B T_e}{\pi m_e}} \exp (\tilde{\phi}_d). \]

Equation 2.36

The normalised Poisson’s equation, for a DC sheath is (equation 2.35):

\[ \frac{\partial^2 \tilde{\Phi}(x)}{\partial \tilde{x}^2} = \tilde{n}_e \left( \tilde{\Phi}(x) \right) - \tilde{n}_i \left( \tilde{\Phi}(x) \right). \]

By inserting the expressions for ion and electron density (2.6 and 2.11, respectively) into this equation, we reach:

\[ \frac{\partial^2 \tilde{\Phi}(x)}{\partial \tilde{x}^2} = \exp (\tilde{\Phi}(x)) - \left( 1 - 2\tilde{\Phi}_{dc} \right)^{-1/2}. \]

This can be integrated by multiplying both sides by \( \partial \tilde{\Phi}/\partial \tilde{x} \). The left-hand side then becomes:

\[ \int \frac{\partial \tilde{\Phi}(x)}{\partial \tilde{x}} \frac{\partial^2 \tilde{\Phi}(x)}{\partial \tilde{x}^2} d\tilde{x} = \frac{1}{2} \left( \frac{\partial \tilde{\Phi}(x)}{\partial \tilde{x}} \right)^2 \]

while the right-hand side becomes:

\[ \int \frac{\partial \tilde{\Phi}(x)}{\partial \tilde{x}} \left[ \exp \left( \tilde{\Phi}(x) \right) - \left( 1 - 2\tilde{\Phi}_{dc} \right)^{-1/2} \right] d\tilde{x} = \int \left[ \exp \left( \tilde{\Phi}(x) \right) - \left( 1 - 2\tilde{\Phi}_{dc} \right)^{-1/2} \right] d\tilde{\Phi} \]

\[ = \exp (\tilde{\Phi}(x)) + \sqrt{1 - 2\tilde{\Phi} + c} \]

where \( c \) is the constant of integration. This can be found using the condition \( \frac{\partial \tilde{\Phi}}{\partial \tilde{x}}|_{\tilde{\Phi}=0} = 0 \), giving \( c = -2 \). Recombining the two sides of this equation then gives equation 2.36:
\[
\frac{1}{\sqrt{2}} \frac{\partial \Phi(x)}{\partial \tilde{x}} = \sqrt{\exp(\Phi)} + \sqrt{1 - 2\Phi - 2}.
\]

**Equation 3.10**

To calculate the electron current in the cutoff velocity distribution model, we begin once more by combining equations 2.21 and 2.22:

\[
I_e(\phi_d) = -e\pi r_d^2 \int \int \int v_o \left(1 + \frac{2e\phi_d}{m_e v_o^2}\right) f_e(v_o) \, d^3v_o.
\]

We then substitute in the electron velocity distribution function. However, the new velocity distribution function (equation 3.2) is no longer isotropic in velocity space.

Here, the integral is given in spherical coordinates, where the velocity \(v_o\) is defined by its magnitude, \(v_o = |v_o|\), and the azimuthal angle \(\theta\), where the \(\theta = 0\) axis points along the x-axis (away from the wall). The distribution remains isotropic in the poloidal angle.

We are considering the case of a dust grain with \(\phi_d > 0\) so, as in the derivation of equation 2.25, there is no minimum approach speed for electrons and we integrate from \(v_o = 0\) to \(\infty\):

\[
f_e(v_o) = n_e \left(\frac{m_e}{2\pi k_B T_e}\right)^{3/2} \exp\left(-\frac{m_e v_o^2}{2k_B T_e}\right) \quad \text{for} \quad v_x < v'_\text{cut}
\]

\[
I_e(\phi_d) = -e\pi r_d^2 \int_{\theta_{\text{min}}}^{\pi} \int \sin(\theta) \, d\theta \, v_o \left(1 + \frac{2e\phi_d}{m_e v_o^2}\right) n_e \left(\frac{m_e}{2\pi k_B T_e}\right)^{3/2} \exp\left(-\frac{m_e v_o^2}{2k_B T_e}\right) 2\pi v_o^2 \, dv_o.
\]

This new variable \(\theta_{\text{min}}(v_o)\) reflects the fact that the cutoff removes electrons with high \(v_x\) and so in spherical coordinates has an angular dependence.

The cutoff criterion,

\[
v'_\text{cut}(x, t) = \sqrt{2e (\phi(x, t) - V_{\text{wall}})} / m_e,
\]

becomes

\[
\theta_{\text{min}} = \arccos\left(\frac{v'_\text{cut}}{v_o}\right) \quad \text{for} \quad v_o > v'_{\text{cut}}
\]
Electrons with a speed \( v_o > v_{\text{cut}} \) cannot also have \( \theta < \theta_{\text{min}} \) as such electrons would have been absorbed by the wall. Electrons with speed \( v_o < v_{\text{cut}} \) cannot reach the wall, and the distribution remains isotropic at these speeds. However, we now have to split the OML integral into two sections:

\[
I_e(\phi_d) = -\frac{e \pi r_d^2}{2} \int_0^{v_{\text{cut}}} \int_0^{\theta_{\text{min}}} \sin(\theta) \, d\theta \, v_o \left( 1 + \frac{2 e \phi_d}{m_e v_o^2} \right) n_e \left( \frac{m_e}{2 \pi k_B T_e} \right)^{3/2} \exp \left( -\frac{m_e v_o^2}{2 k_B T_e} \right) \frac{2 \pi v_o^2}{v_o} \, dv_o
\]

\[
-\frac{e \pi r_d^2}{2} \int_{v_{\text{cut}}}^{v_{\text{cut}} \theta_{\text{min}}} \int_0^{\pi} \sin(\theta) \, d\theta \, v_o \left( 1 + \frac{2 e \phi_d}{m_e v_o^2} \right) n_e \left( \frac{m_e}{2 \pi k_B T_e} \right)^{3/2} \exp \left( -\frac{m_e v_o^2}{2 k_B T_e} \right) \frac{2 \pi v_o^2}{v_o} \, dv_o.
\]

Evaluating the integral in theta gives:

\[
\int_0^{\pi} \sin(\theta) \, d\theta = 2, \quad \int_{\theta_{\text{min}}}^{\pi} \sin(\theta) \, d\theta = -\left( \cos(\theta) \right)_{\theta_{\text{min}}}^{\pi} = \frac{v_{\text{cut}}}{v_o} + 1.
\]

This can then be inserted into the OML integral:

\[
I_e(\phi_d) = -2 n_e e \pi r_d^2 \left( \frac{m_e}{2 \pi k_B T_e} \right)^{3/2} \left[ \int_0^{v_{\text{cut}}} 2 v_o \left( 1 + \frac{2 e \phi_d}{m_e v_o^2} \right) \exp \left( -\frac{m_e v_o^2}{2 k_B T_e} \right) \frac{v_o^2}{v_o} \, dv_o \right]
\]

\[
+ \int_{v_{\text{cut}}}^{v_{\text{cut}} \theta_{\text{min}}} \left( \frac{v_{\text{cut}}}{v_o} + 1 \right) v_o \left( 1 + \frac{2 e \phi_d}{m_e v_o^2} \right) \exp \left( -\frac{m_e v_o^2}{2 k_B T_e} \right) \frac{v_o^2}{v_o} \, dv_o \right].
\]

As done in the derivation of equations 2.24 and 2.25 above, we substitute in the following normalised variables: \( \tilde{v} = \frac{v}{\sqrt{k_B T_e/m_e}} \) and \( \tilde{\phi}_d = e \phi_d/(k_B T_e) \).
\[ I_e (\phi_d) = -2n_e e \pi^2 r_d^2 \left( \frac{m_e}{2\pi k_B T_e} \right)^{3/2} \left( \frac{k_B T_e}{m_e} \right)^2 \left[ \int_0^{\tilde{v}_{\text{cut}}} 2\tilde{v}_o \left( 1 + \frac{2\phi_d}{\tilde{v}_o^2} \right) \exp \left( -\frac{\tilde{v}_o^3}{2} \right) \tilde{v}_o d\tilde{v}_o \right. \\
\left. + \int_{\tilde{v}_{\text{cut}}}^{\infty} \left( \frac{\tilde{v}'_{\text{cut}}}{\tilde{v}_o} + 1 \right) \tilde{v}_o \left( 1 + \frac{2\phi_d}{\tilde{v}_o^2} \right) \exp \left( -\frac{\tilde{v}_o^3}{2} \right) \tilde{v}_o d\tilde{v}_o \right] . \]

This simplifies to:

\[ I_e (\phi_d) = -n_e e \pi r_d^2 \sqrt{\frac{k_B T_e}{2\pi m_e}} \left[ \int_0^{\tilde{v}_{\text{cut}}} 2 \left( 1 + \frac{2\phi_d}{\tilde{v}_o^2} \right) \exp \left( -\frac{\tilde{v}_o^3}{2} \right) \tilde{v}_o^3 d\tilde{v}_o \right. \\
\left. + \int_{\tilde{v}_{\text{cut}}}^{\infty} \left( \frac{\tilde{v}'_{\text{cut}}}{\tilde{v}_o} + 1 \right) \left( 1 + \frac{2\phi_d}{\tilde{v}_o^2} \right) \exp \left( -\frac{\tilde{v}_o^3}{2} \right) \tilde{v}_o^3 d\tilde{v}_o \right]. \]

Once more, we apply a set of standard integrals:

\[ \int_0^a x \exp \left( -\frac{x^2}{2} \right) dx = 1 - \exp \left( -\frac{a^2}{2} \right), \]

\[ \int_0^a x^3 \exp \left( -\frac{x^2}{2} \right) dx = 2 - (a^2 + 2) \exp \left( -\frac{a^2}{2} \right), \]

\[ \int_a^\infty x^3 \exp \left( -\frac{x^2}{2} \right) dx = (a^2 + 2) \exp \left( -\frac{a^2}{2} \right), \]

\[ \int_a^\infty x^2 \exp \left( -\frac{x^2}{2} \right) dx = a \exp \left( -\frac{a^2}{2} \right) + \sqrt{\frac{\pi}{2}} \text{erfc} \left( \frac{a}{\sqrt{2}} \right), \]

\[ \int_a^\infty x \exp \left( -\frac{x^2}{2} \right) dx = \text{erfc} \left( \frac{a}{\sqrt{2}} \right), \quad \int_a^\infty \exp \left( -\frac{x^2}{2} \right) dx = \sqrt{\frac{\pi}{2}} \text{erfc} \left( \frac{a}{\sqrt{2}} \right). \]
Giving the following rather long equation:

\[
I_e(\phi_d) = -n_e e \pi r_d^2 \sqrt{\frac{k_B T_e}{2 \pi m_e}} \left[ 4 - 2 \left( \tilde{v}_{\text{cut}}^2 + 2 \right) \exp \left( -\frac{\tilde{v}_{\text{cut}}^2}{2} \right) + 4 \tilde{\phi}_d \left( 1 - \exp \left( -\frac{\tilde{v}_{\text{cut}}^2}{2} \right) \right) \\
+ \left( \tilde{v}_{\text{cut}}^2 + 2 \right) \exp \left( -\frac{\tilde{v}_{\text{cut}}^2}{2} \right) + \tilde{v}_{\text{cut}} \left( \tilde{v}_{\text{cut}} \exp \left( -\frac{\tilde{v}_{\text{cut}}^2}{2} \right) + \sqrt{\frac{\pi}{2}} \text{erfc} \left( \frac{\tilde{v}_{\text{cut}}}{\sqrt{2}} \right) \right) \\
+ 2 \tilde{\phi}_d \exp \left( -\frac{\tilde{v}_{\text{cut}}^2}{2} \right) + 2 \tilde{\phi}_d \tilde{v}_{\text{cut}}' \sqrt{\frac{\pi}{2}} \text{erfc} \left( \frac{\tilde{v}_{\text{cut}}}{\sqrt{2}} \right) \right].
\]

This can be tidied up to give equation 3.10:

\[
I_e(\phi_d) = -n_e e \pi r_d^2 \sqrt{\frac{k_B T_e}{2 \pi m_e}} \left[ 4 + 4 \tilde{\phi}_d + \sqrt{\frac{\pi}{2}} \tilde{v}_{\text{cut}} \left( 1 + 2 \tilde{\phi}_d \right) \text{erfc} \left( \frac{\tilde{v}_{\text{cut}}}{\sqrt{2}} \right) \\
- \exp \left( -\frac{\tilde{v}_{\text{cut}}^2}{2} \right) \left( 2 + 2 \tilde{\phi}_d \right) \right].
\]
Appendix B: Additional Figures

Figures 4.7 and 4.8: separate grain potentials

In figures 4.7 and 4.8, the grain potentials given by the CC model are only shown as a fraction of those predicted by the BE model. Here, they are shown separately for further information.

Figure B.1: Dust grain potential for $\tilde{V}_{rf} = 100$ and 200, for both BE and CC models (denoted by solid and dashed lines respectively).
Figure 4.9: force breakdown

The separate forces - electrostatic ($F_e$), ion drag ($F_{id}$), and gravity ($F_g$) - acting on a 5\(\mu\)m dust grain in an RF driven sheath ($\tilde{V}_{rf} = 50$). This is a breakdown of forces for the same parameters as figure 4.9, in which only the total force is given.

Figure B.2: Individual forces (electrostatic, gravitational, and ion drag) exerted on a 5 \(\mu\)m dust grain in the RF sheath ($\tilde{V}_{rf} = 50$) evaluated using CC model.

Figures 4.9 and 4.10: underlying force profile

The force profile for a 10 \(\mu\)m dust grain in an RF sheath with driving voltage $\tilde{V}_{rf} = 200$. The different force profiles given by the BE and CC models have already addressed by
the dust-grain force profiles shown in Chapter 4 (figures 4.9 and 4.10). However, this particular case is illustrative in order to compare the dust grain dynamics in figures 4.11 and 4.12, which use the same parameters.

Figure B.3: Normalised force exerted on a 10μm dust grain in the RF sheath ($\tilde{V}_{rf} = 200$) for BE and CC models (denoted by solid and dashed lines respectively).
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