ION TRAJECTORIES AT COLLISIONLESS SHOCKS IN SPACE PLASMAS

by
Philip Ryan Newman

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Abstract

The thesis investigates ion behaviour at collisionless shocks, with a focus on two areas of interest.

The first area concerns the reflection of particles from collisionless shocks, a necessary mechanism for thermalization at a shock at sufficiently high Mach numbers such as ordinarily prevail at the Earth's bow shock. Previous studies have examined the trajectories of reflected ions with the assumption of a planar shock. In this study, a general framework is developed to describe the trajectory of an ion after reflection, with application to a variety of shock geometries. The conditions allowing an ion to return to the shock after reflection and to return with an increased normal velocity are studied, with three primary parameters considered: the radius of curvature, the magnetic field orientation, and the incident velocity in the shock normal direction. Each of these parameters depends on the shape of the shock and the location of incidence. Results are reported for cylindrical, spherical, and parabolic shock geometries, over ranges of shock curvatures, magnetic field orientations, and incident velocities.

Second, we consider the thermalization of the ion distribution initially transmitted through the shock under low Mach number conditions, where reflection is a less significant contributor to thermalization. Previous work has considered the phase area invariant in an exactly perpendicular case. This is generalized to a quasi-perpendicular shock, and invariants of the flow are determined for a Hamiltonian formulation. The evolution of the distribution through the shock is then studied analytically and numerically. Results regarding the shape of phase shells of constant probability, the phase volume within these shells, and the temperature of the distribution are given.
Acknowledgements

I wish to thank my supervisors, Dr Steve Ellacott and Dr Will Wilkinson, without whose guidance and support this thesis would not have been possible. They have always been available as required to overcome questions and obstacles in my research, and I am very grateful for their generosity.

I also thank all the members of the School of Computing, Engineering, and Mathematics at the University of Brighton, who have provided a friendly working atmosphere during my time there, as well as access to all the necessary facilities and resources at the School.

Finally, I wish to thank all my relatives and friends, especially my parents, John and Deborah Newman, my sister, Elizabeth Ables, and my flatmate, Sarah Bargiela, for their love and encouragement.
Declaration

I declare that the research contained in this thesis, unless otherwise formally indicated within the text, is the original work of the author. The thesis has not been previously submitted to this or any other university for a degree, and does not incorporate any material already submitted for a degree.

Signed

Dated
18/2/13
To my parents,
John and Deborah
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Chapter 1

Introduction

When a supersonic plasma flow, such as the solar wind, encounters an obstacle in its path, a shock wave may arise where the flow is slowed and deflected around the obstacle. The low density of space plasmas means that the heating that accompanies the deceleration of the flow at the shock is accomplished without collisions between the particles in the flow, in contrast to what happens at shocks in dense gases such as the Earth's atmosphere. Instead, it is the electric and magnetic properties of the ionized solar wind plasma which makes collisionless shocks possible [Sagdeev and Kennel, 1991].

The interaction between electromagnetic fields and particles in the plasma results in a variety of phenomena at collisionless shocks, including particle acceleration, wave generation, and wave-particle interactions. Of particular interest is the effect of the shock on the positive ions, which are the main momentum and energy carriers in the solar wind. This thesis investigates two aspects of the interaction between the ions and a collisionless shock, first focusing on the reflection of ions - a contributor to thermalization at high Mach number shocks - for non-planar shock geometries, and then considering the thermalization of the transmitted ions for low Mach number, quasi-perpendicular planar shocks.

This introductory chapter aims to provide a brief overview of the field, including a review of the theoretical, computational, and observational results forming the foundation for the original research described in subsequent chapters.
1.1 The Solar Wind Plasma

The solar wind is a plasma, an ionized fluid composed primarily of electrons and protons (with some larger positive ions). This fluid travels outwardly from the Sun and through the solar system as a result of coronal expansion. For typical temperatures (about $10^6$ K) within the corona of the Sun, nearly half of the electrons have the necessary thermal velocity to escape the gravitational pull of the star, while only a small fraction of the ions do. This would result in a charge imbalance, but a large electric field is generated to maintain charge neutrality, pushing the ions outward [Parks, 2003].

This section discusses properties of plasmas in general, as well as typical parameters for the solar wind plasma in particular and the solar wind's suitability as a plasma laboratory. We are especially interested in the solar wind's properties at 1 Astronomical Unit (AU), the distance between the Sun and the Earth, as our primary focus will be on the behaviour of the solar wind at the Earth's bow shock. We will then discuss several methodologies used to study the behaviour of plasmas, which will form the foundation for a discussion of the Earth's bow shock in Section 1.2 as well as to the remainder of the thesis.

1.1.1 Properties of the Solar Wind Plasma

One important feature of a plasma which is absent in a neutral fluid is Debye shielding, which is a result of the charges of individual plasma particles. Consider a solitary ion in a vacuum. At a distance $r$ from this source ion, the charge results in an electric potential, $\psi(r)$, and the equation for this potential can be determined using a Poisson equation:

$$\nabla^2 \psi(r) = -\frac{\rho}{\epsilon_0} \quad (1.1)$$

where $\rho$ is the charge density and $\epsilon_0$ is the permittivity of free space. (This equation can be derived from Gauss's law, which will be introduced in Section 1.1.2.) In the case of a point charge, $\rho$ is zero at all points except $r = 0$, and the solution to the equation is:
where $q$ is the charge of the particle. However, in a plasma, the particle is partially shielded by particles of the opposite charge. For example, a proton attracts electrons to its close proximity, and these electrons counteract the electrostatic potential of the proton. As a result, it is no longer true that the charge density is zero in the vicinity of the test charge. Assuming the electrons are in thermal equilibrium, it is possible to modify equation (1.1) to account for the increased electron density attracted to the test charge [e.g., Cravens, 1997], and the solution to the resulting equation is:

$$
\psi = \frac{q}{4\pi \varepsilon_0 r} \exp \left( - \frac{r}{\lambda_D} \right)
$$

(1.3)

The parameter governing this shielding is the Debye length, $\lambda_D$:

$$
\lambda_D^2 = \frac{k_B T_e \varepsilon_0}{n_0 q_e^2}
$$

(1.4)

where $k_B$ is the Boltzmann constant, $T_e$ is the electron temperature, and $n_0$ is a "reference" density equal to both the ion and electron densities [Cravens, 1997]. From equation (1.3), we can see that near the particle ($r \ll \lambda_D$), the exponential approaches 1, and the potential therefore approximates that due to an ion in a vacuum. However, away from the test charge ($r \gg \lambda_D$), the exponential goes to 0 - while the potential in a vacuum also goes to 0 as $r$ increases, the shielded potential does so much faster. As a consequence, the Coulomb force in a plasma is short range, only affecting other particles on the scale of the Debye length.

From the Debye length and the density of the particles, we can determine whether it is appropriate to treat a given fluid as a plasma. The plasma parameter, $g$, is defined by:

$$
g = \frac{3}{4\pi n_0 \lambda_D^3}
$$

(1.5)
which is the reciprocal of the number of ions within a “Debye Sphere” (a sphere with radius $\lambda_D$). If $g \ll 1$, the number of particles in a Debye sphere is large enough to apply statistical concepts, and Debye shielding is meaningful. The plasma parameter is a measure of interparticle interactions; for small $g$, the interparticle potential energy is small relative to the kinetic energy, and thus the plasma can be approximated as an ideal gas. (The plasma parameter is sometimes defined in the literature as the reciprocal of $g$.)

Also used to characterize plasmas is the plasma beta, $\beta$, which quantifies the importance of kinetic vs. electromagnetic behaviour. The plasma beta is the ratio between the plasma pressure and the magnetic pressure:

$$\beta = \frac{P}{B} = \frac{n k_B T}{\mu_0 B^2}$$  \hspace{1cm} (1.6)

where $B$ is the strength of the magnetic field and $\mu_0$ is the vacuum permeability constant. Typically, the solar wind is categorized as either a low $\beta$ (cold) plasma, when $\beta \ll 1$, or a high $\beta$ (warm) plasma.

Other important plasma parameters are the characteristic plasma frequencies. As a response to any charge imbalance, the electrostatic forces in the plasma act on the electrons to restore charge neutrality, resulting in oscillations about the equilibrium. The characteristic frequency of these oscillations depends on the thermal speed and the Debye length [Boyd and Sanderson, 2003], and for the electrons is given by:

$$\omega_{pe} = \sqrt{\frac{\frac{k_B T_e}{m_e}}{\lambda_D}} = \sqrt{\frac{n_e q_e^2}{m_e e_0}}$$  \hspace{1cm} (1.7)

where $m_e$ is the electron mass. Likewise, the ion plasma frequency is:

$$\omega_{pi} = \sqrt{\frac{n_i q_i^2}{m_i e_0}}$$  \hspace{1cm} (1.8)
Since the ions are much more massive than the electrons, the ion plasma frequency is significantly lower than the electron plasma frequency. This can be an important consideration for simulation algorithms, which must address the effect this disparity in time scales can have on stability.

Table 1.1 gives a selection of average solar wind properties at 1 AU obtained via space observations. Table 1.2 gives typical values for the derived plasma properties discussed in this section, determined by the other macroscopic parameters of the plasma found in Table 1.1. For the solar wind, the Debye length is typically on the same scale or larger than a probe that might be used to take measurements. This allows the spacecraft to study individual particle behaviour without interference from, and without disturbing, the plasma [Schwartz, 1985].

Because of its low density, the solar wind is a collisionless plasma - the collisional mean free path of an ion (a measure of the distance traveled by a particle between collisions) is on the order of 1 AU, whereas the scales we are interested in are much smaller [e.g., Burgess, 1995]. In contrast, the collisional mean free path in air is on the order of 1 micrometer [Sagdeev and Kennel, 1991], due to air's greater density.

1.1.2 Maxwell's Equations and Particle Motion

A plasma is composed of charged particles; the solar wind consists mostly of protons and electrons, with some heavier ions. The motion of these particles is governed by the electromagnetic fields generated by the Sun, any nearby planetary body, and the other solar wind particles. The relationship between the charged particles and the electromagnetic fields is expressed through Maxwell's equations and the Lorentz equation [e.g., Boyd and Sanderson, 2003]. Maxwell's equations are Gauss' law:

\[ \nabla \cdot \mathbf{E} = \frac{q}{\varepsilon_0} \]  

(1.9)

governing the relationship between the electric field and the charge distribution; Gauss' law for magnetism:
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density ($n$)</td>
<td>$5\text{cm}^{-3}$</td>
</tr>
<tr>
<td>Velocity ($V_{sw}$)</td>
<td>$300 - 800\text{km/s}$</td>
</tr>
<tr>
<td>Temperature ($T$)</td>
<td>$10^5\text{K}$</td>
</tr>
<tr>
<td>Magnetic field ($</td>
<td>B</td>
</tr>
</tbody>
</table>

Table 1.1: Selected typical solar wind parameters at the Earth (1 AU) to one significant figure. Values from Schwartz [1985], based on statistical survey from Feldman et al. [1977].
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Debye Length ($\lambda_D$)</td>
<td>$10\text{m}$</td>
</tr>
<tr>
<td>Plasma Parameter ($g$)</td>
<td>$10^{-10}$</td>
</tr>
<tr>
<td>Ion Plasma Beta ($\beta_i$)</td>
<td>$0.5 - 1$</td>
</tr>
<tr>
<td>Mean Free Path ($\lambda_{mfp}$)</td>
<td>$0.6\text{AU}$</td>
</tr>
<tr>
<td>Ion Plasma Frequency ($\omega_{pi}$)</td>
<td>$3000\text{rad/s}$</td>
</tr>
<tr>
<td>Electron Plasma Frequency ($\omega_{pe}$)</td>
<td>$10^5\text{rad/s}$</td>
</tr>
<tr>
<td>Ion Cyclotron Frequency ($\Omega_{ci}$)</td>
<td>$0.5\text{rad/s}$</td>
</tr>
</tbody>
</table>

Table 1.2: Selected typical plasma parameters in the solar wind at the Earth (1 AU) to one significant figure, derived from properties observed in Table 1.1. Value for $g$ from Cravens [1997], other values from Schwartz [1985], based on statistical survey from Feldman et al. [1977].
\[ \nabla \cdot \mathbf{B} = 0 \]

(1.10)

which states that there is no comparable single "magnetic charge" (monopole), and thus the magnetic flux through any closed surface is 0; Faraday's law:

\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \]

(1.11)

which relates the electric field to time changes in the magnetic field; and Ampere's law:

\[ \nabla \times \mathbf{B} = \varepsilon_0 \mu_0 \frac{\partial \mathbf{E}}{\partial t} + \mu_0 \mathbf{J} \]

(1.12)

which relates the magnetic field to the change in the electric field and the current.

Together with the equation of motion for the particles, we have a complete system describing the behaviour of both the particles and the fields. However, Maxwell's equations show that the electromagnetic fields depend on the charge distribution and current due to individual charged particles in the plasma, and the resulting many-body system is analytically intractable - we cannot solve exactly for all of the positions and velocities of the particles simultaneously, or calculate the fields exactly in a self-consistent manner. Thus, in order to investigate the behaviour of a collection of charged particles in the presence of electromagnetic fields, we must simplify the set of equations.

In this section, we solve the equations by assuming static or otherwise simplified field models, rather than using Maxwell's equations to solve for the fields self-consistently; in later sections, we will investigate other alternatives to approaching these equations.

We first consider the motion of an ion in the presence of uniform electromagnetic fields, which is governed by the Lorentz equation of motion. The Lorentz force on a particle of charge \( q \) and mass \( m \) is:
\[
F = m \frac{dv}{dt} = q(E + v \times B)
\]  \hspace{1cm} (1.13)

We will assume for the moment that \(E\) and \(B\) are orthogonal, for reasons which will be discussed later in the section. Consider the unit vectors \(\mathbf{b} = \frac{\mathbf{B}}{|\mathbf{B}|}\) and \(\mathbf{e} = \frac{\mathbf{E}}{|\mathbf{E}|}\), along with a third unit vector \(\mathbf{k} = \mathbf{e} \times \mathbf{b}\). Note that in the \(\mathbf{b}\)-direction, the force is 0 (i.e., \(v_b\) is constant). We can solve for the remaining velocity components as a system of differential equations:

\[
\frac{dv_e}{dt} = \frac{|E| - |B|v_k}{\dot{m}}
\]  \hspace{1cm} (1.14)

\[
\frac{dv_k}{dt} = \frac{|B|v_e}{\dot{m}}
\]  \hspace{1cm} (1.15)

where \(\dot{m} = \frac{m}{q}\). Differentiating one equation and substituting into the other decouples the equations:

\[
\frac{d^2v_e}{dt^2} = -\left(\frac{|B|}{\dot{m}}\right)^2 v_e
\]  \hspace{1cm} (1.16)

\[
\frac{d^2v_k}{dt^2} = -\left(\frac{|B|}{\dot{m}}\right)^2 v_k + \frac{|B||E|}{\dot{m}^2}
\]  \hspace{1cm} (1.17)

The general solution to these equations is:

\[
v_e = C\cos(\Omega_v t + \alpha)
\]  \hspace{1cm} (1.18)

\[
v_k = C\sin(\Omega_v t + \alpha) + \frac{|E|}{|B|}
\]  \hspace{1cm} (1.19)
where $C$ and $\alpha$ are constants of integration to be determined by initial conditions and $\Omega_{ci} = \frac{qB}{m_i}$ is the gyrofrequency (ion cyclotron frequency).

Thus, in the presence of a constant magnetic field and no electric field, the motion of the particle is circular in the plane perpendicular to the magnetic field and constant parallel to the magnetic field, resulting in helical motion (or circular, if $v_\parallel = v_b = 0$). The circular motion in the plane perpendicular to the magnetic field is determined by the parameters $\Omega_{ci}$ and $v_\perp = \sqrt{v_\perp^2 + v_\parallel^2} = C$, which depend on the initial conditions. The gyroperiod (the time it takes for the ion to complete one "Larmor orbit") is $\frac{2\pi}{\Omega_{ci}}$, while the gyroradius ("Larmor radius") is $\frac{v_\perp}{\Omega_{ci}}$.

In the case of a constant electric field perpendicular to the magnetic field, we obtain a drift velocity in the direction orthogonal to both fields: $v_d = \frac{E_v}{|E|} \hat{k}$. Because of the direction of this drift motion, it is often called the $E \times B$ drift.

We now consider a constant electric field in the direction parallel to the magnetic field. This electric field applies a constant force to the particle in the $\hat{b}$-direction, which means relativistic effects would need to be taken into account for a single particle in fixed fields (the particle will continue to gain velocity, in the absence of other forces). In a realistic plasma (with a collection of particles, rather than a single test particle), since the direction of the force depends on the charge, a non-zero $E_\parallel$ would result in charge separation and large currents, which in turn would produce an $E_\parallel$ cancelling out the original. Since the studies in the thesis assume static, homogeneous, equilibrium fields, we will assume $E_\parallel = 0$; for non-equilibrium fields, however, the value of $E_\parallel$ may oscillate about zero.

For a more general field profile, we must solve the Lorentz equation for the particle motion numerically. However, if the inhomogeneity in the fields is small, such that the field experienced by a particle over a single orbit is almost constant, the motion can be approximated by a perturbative approach first used by Alfvén, known as the guiding centre approximation. The guiding centre method uses a first order approximation to the magnetic field:

$$
B(r) \approx B(r_0) + [(r - r_0) \cdot \nabla] B|_{r=r_0}
$$

(1.20)

where $r_0$ is the position of the guiding centre. Thus, changes in the magnetic field over a Larmor orbit (a single gyroperiod) are averaged out.
In general, the spatial changes in the magnetic field can be represented by the partial derivatives, $\frac{\partial B}{\partial x}$, and changes in each field component over each spatial direction can give rise to different "drift" velocities (similar to the $E \times B$ drift which appears for a constant non-zero electric field) called "gradient drift" and "curvature drift", depending on the source of the inhomogeneity. Littlejohn [1979] details a rigorous method for applying the guiding centre approximation to a Hamiltonian system.

### 1.1.3 Approximate Invariance of the Magnetic Moment

While throughout the thesis we assume that the magnetic field is time-independent (and in Chapter 2, constant in space as well), in reality the magnetic field profile varies in both space and time. If we assume that the magnetic field varies slowly in time (i.e., the change in the magnetic field strength relative to the magnitude of the field is negligible over a gyroperiod), we can find certain "adiabatic invariants". These are approximate constants of motion, and their consideration provides interesting insights on the behaviour of particles in a plasma, as well as providing justification for simplifications made to the magnetic field models used.

The most prominent of these approximate invariants is the magnetic moment of a gyrating ion [Boyd and Sanderson, 2003]. It is a measure of the magnetic flux created by the charged, gyrating particle in the presence of a magnetic field; strictly speaking, the magnetic moment is a diamagnetic vector (opposite in direction to the magnetic field), but here we are only concerned with its magnitude, which is given by the kinetic energy of the particle due to gyration divided by the magnetic field strength:

$$\mu_B = \frac{m|v_\perp|^2}{2B} \quad (1.21)$$

Starting with a magnetic field which is constant in space but not time, we first note that the changing magnetic field induces an electric field such that $v_\perp$ is no longer constant. Multiplying the Lorentz equation (1.13) by $v_\perp$ we have:

$$\frac{d}{dt} \left( \frac{1}{2}mv_\perp \cdot v_\perp \right) = qE \cdot v_\perp \quad (1.22)$$
Over a single Larmor orbit, the particle’s energy changes by:

\[
\partial \left( \frac{1}{2} mv_\perp^2 \right) = \oint \mathbf{E} \cdot \mathbf{d}r_\perp \\
= q \int (\nabla \times \mathbf{E}) \cdot \mathbf{d}S
\]  

(1.23)  

(1.24)

where \( \mathbf{d}r_\perp = \mathbf{v}_\perp \, dt \) and \( \mathbf{d}S \) is a surface element enclosed by the orbit of the ion. Note that by “orbit” here we mean the oscillatory motion about the guiding centre of the trajectory. In general, the motion of the particle is helical, not circular, but if the change in the fields over a gyroperiod is negligible, we can ignore the motion of the guiding centre in averaging over a gyroperiod. Now:

\[
\partial \left( \frac{1}{2} mv_\perp^2 \right) = -q \int \frac{\partial \mathbf{B}}{\partial t} \cdot \mathbf{d}S
\]  

(1.25)

by Faraday’s law. Since the field changes slowly:

\[
\partial \left( \frac{1}{2} mv_\perp^2 \right) \approx \pi r_L^2 q \dot{B} \\
= \frac{mv_\perp^2}{2} \frac{2\pi \dot{B}}{|\Omega| B} \\
= \frac{mv_\perp^2}{2} \frac{\partial B}{B}
\]  

(1.26)

where \( \pi r_L^2 \) is the area enclosed by the Larmor orbit, which is expressed in terms of the particle velocity perpendicular to the magnetic field, \( \dot{B} = \frac{dB}{dt} \), and \( \partial B \) is the change in the magnetic field strength over one gyroperiod. The relative change in the kinetic energy of the particle and the relative change in the magnetic field strength are therefore equivalent:

\[
\frac{\partial \left( \frac{1}{2} mv_\perp^2 \right)}{\frac{1}{2} mv_\perp^2} = \frac{\partial B}{B}
\]  

(1.27)

Thus, the ratio of the two quantities must remain constant, and since this ratio is the magnetic moment, we are left with the invariance of the magnetic moment:
The magnetic moment is also conserved for inhomogeneous fields (again assuming that they change slowly relative to the gyrofrequency), by a similar averaging argument. Appendix A offers an alternate derivation, showing that the magnetic moment is an approximation of the Poincaré-Cartan integral invariant, as are the other adiabatic invariants discussed there.

A consequence of the approximate invariance of the magnetic moment is the concept of magnetic mirrors. Consider a particle traveling toward a region of increased field strength. As $B$ increases, the kinetic energy of the particle perpendicular to the field must also increase, since the ratio of these quantities (the magnetic moment) is constant. However, because of the conservation of energy, it may be the case that the magnetic field strength increases to the point that $v = 0$. Thus, the particle is reflected by the strength of the magnetic field. Whether or not a given ion will be reflected by a magnetic mirror depends on the ratio of maximum and minimum field strengths, as well as the “pitch angle”, the angle between the particle trajectory and the magnetic field [Boyd and Sanderson, 2003].

At a shock, the invariance of the magnetic moment breaks down, due to the abrupt change in the magnetic field strength. The assumption that the magnetic field changes slowly on the scale of the ion gyroradius and gyropedon may also be invalid due to turbulence (in the ion foreshock, for example). However, where these assumptions are valid, the invariance of the magnetic moment is important in understanding the motion of the ions.

\[
\frac{\partial (\mu_B)}{\partial t} = 0
\]  

(1.28)

1.1.4 The Solar Wind as a Fluid

One difficulty in studying the behaviour of a plasma is that the charged particles in the plasma induce electromagnetic fields, in addition to the external fields generated by, for example, the Sun or a planetary body. These particle fields may be significant in determining the trajectories of the particles, as the ions and electrons attract and repel each other.

Simulations which take into account the fields generated by the ions (and electrons) self-consistently exist, and will be discussed later in this chapter.
However, alternative methods are also used to study plasma behaviour. Rather than treating the particles individually, in Magnetohydrodynamics (MHD) the plasma is treated as a fluid and the electromagnetic fields are generated by this fluid, approximating the effects of the particles on the fields [Boyd and Sanderson, 2003].

Although the research presented in the following chapters focuses on individual particles and particle distributions (i.e., kinetic effects), it is useful to compare results with the predictions of MHD. For example, when discussing shocks reference is often made to the Rankine-Hugoniot relations (see Section 1.2.2) arising from MHD, which express the requirement that, ultimately, a shock must conserve mass, momentum, and energy.

**Fluid Mechanics**

We begin with the equations for the motion of a fluid, from fluid dynamics, following Boyd and Sanderson [2003]. These equations relate the quantities $\rho$ (density), $u$ (velocity), $P$ (pressure), and $T$ (temperature), which are all functions of position and time.

For a given quantity, $F$, following a fluid element with flow velocity $v = u(r, t)$, we use the “convective” derivative, $\frac{D F}{D t}$, in place of the usual time derivative. The convective derivative expresses changes in both time and space:

$$\frac{D F}{D t} \equiv \frac{\partial F}{\partial t} + u \cdot \nabla F \quad (1.29)$$

Consider a fluid volume enclosed by a surface, $A$, with mass density $\rho$. The total mass enclosed is $\int_V \rho dV$, while the rate at which mass flows outward through the surface is $\int_A \rho u \cdot dA$. Thus:

$$\frac{d}{dt} \int_V \rho dV = -\int_A \rho u \cdot dA \quad (1.30)$$

By the Divergence theorem, we can relate the right-hand side to a volume integral, and obtain, after rearrangement:
\[ \int_V \left[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) \right] dV = 0 \]  
\hspace{2cm} (1.31)

Since this is true for any volume in the fluid, the integrand is 0, and from this follows the equation of continuity (conservation of mass):

\[ \frac{D\rho}{Dt} = -\rho(\nabla \cdot u) \]  
\hspace{2cm} (1.32)

In deriving the equation of motion for a fluid element, we can separate long range forces (represented by \( F \), the force per unit mass) which are the same for all particles in the element, and short range forces which affect the momentum at the surface of the fluid element. The latter force per unit area - stress - is given by the stress tensor \( \Phi \), where the components \( \Phi_{ij} \) give the i-component of the force on the unit area normal to the j-direction. In differential form, this results in the equation:

\[ \frac{\rho Du_i}{Dt} = \rho F_i + \frac{\partial \Phi_{ij}}{\partial r_j} \]  
\hspace{2cm} (1.33)

For an isotropic fluid at rest, the off-diagonal elements of the stress tensor are zero, and \( \Phi_{ij} = -P \delta_{ij} \) where \( P \) is the thermodynamic pressure and \( \delta_{ij} \) is the Kronecker delta. However, this is not true for a fluid in motion, nor is it true for a magnetized plasma. The non-isotropic part of the stress tensor is called the “viscous stress tensor” and we have, for a fluid in motion:

\[ \Phi_{ij} = -P \delta_{ij} + \mu \left( \frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i} - \frac{2}{3} \delta_{ij} \nabla \cdot u \right) \]  
\hspace{2cm} (1.34)

where \( \mu \) is the coefficient of viscosity. After substitution, the equation of motion becomes:

\[ \rho \frac{Du_i}{Dt} = \rho F_i - \frac{\partial P}{\partial r_i} + \frac{\partial}{\partial r_j} \left[ \mu \left( \frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial r_k} \right) \right] \]  
\hspace{2cm} (1.35)

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The system is closed with an equation for $P$, which is equivalent to the conservation of energy:

\[
\frac{DP}{Dt} = -\gamma P \nabla \cdot u + (\gamma - 1) \nabla \cdot (\kappa \nabla T) + \frac{\gamma - 1}{\sigma} j^2 \\
+ (\gamma - 1) \mu \left( \frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i} - \frac{2}{3} \delta_{ij} \nabla \cdot u \right) \frac{\partial u_i}{\partial r_j}
\]  

(1.36)

where $\kappa$ is the coefficient of heat conduction and $\gamma = \frac{cp}{cv}$ is the ratio between the constant pressure and constant volume heat capacities.

There are any number of additional "state" variables which may appear; however, we can write any of them in terms of $P$ and $\rho$, so we have an "equation of state" for each of these variables. Since the temperature, $T$, appears in the previous equation, we require the equation of state for $T$, which is the ideal gas law:

\[
P = R_0 \rho T
\]

(1.37)

where $R_0$ is the gas constant. This completes the fluid equations.

**Ideal MHD**

The primary difference between the fluid description of a plasma and that of a neutral fluid is that a plasma consists of two (or more) species with opposite charges and different masses which interact through electric attraction and repulsion. However, even ignoring this force can provide a meaningful one-fluid magnetohydrodynamic model, with the magnetic force acting on the fluid as an additional variable compared to the neutral fluid case.

To obtain the one-fluid MHD equations, we specify that the force, $F$, appearing in the equation of motion is the electromagnetic Lorentz force, with the fields determined by Maxwell’s equations. After some simplification, we find that we can eliminate the current and electric field, and thus only require one additional equation, the induction equation for the magnetic field, $B$: 

28
\[ \frac{\partial \mathbf{B}}{\partial t} = \frac{1}{\sigma \mu_0} \nabla^2 \mathbf{B} + \nabla \times (\mathbf{u} \times \mathbf{B}) \]  

(1.38)

where \( \sigma \) is a resistive term (treated as a constant here) from Ohm's law. Boyd and Sanderson [2003] note that the form of Ohm's law used in a one-fluid model - \( \mathbf{J} = \sigma(\mathbf{E} + \mathbf{u} \times \mathbf{B}) \) - should be regarded as a model equation selected for mathematical simplicity. A more rigorous MHD treatment requires a two-fluid model.

At this point, the system of equations is complete, but various simplifications are usually made to make them suitable for general use. The most commonly used form of MHD is Ideal MHD, where the equations are simplified by ignoring all dissipation. This is equivalent to letting the scale length tend to infinity. In Ideal MHD, the energy equation is the adiabatic gas law:

\[ \frac{D(P \rho^{-\gamma})}{Dt} = 0 \]  

(1.39)

while the induction equation simplifies to:

\[ \frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{u} \times \mathbf{B}) \]  

(1.40)

Ideal MHD relies on strong collisions within the fluid (which allow the particle distributions to remain roughly Maxwellian), but, as noted previously, shocks such as the bow shock are collisionless and occur on a smaller spatial scale than can be modelled by MHD. Because of this, MHD is not suitable for studying the kinetic behaviour within a plasma through a collisionless shock. However, MHD is useful for studying larger scale properties of the flow. Fluid theory predicts, for example, the necessity of a change in the nature of dissipation above a "critical" Mach number: for supercritical shocks, there is no continuous solution in Resistive MHD, and ion viscosity (caused by the reflection of a portion of the distribution) must be included [Thomsen et al., 1985 and references therein].
MHD Waves

With the MHD equations from the previous section, we can investigate the behaviour of a collection of charged particles in the presence of electromagnetic fields and determine how the bulk properties of the plasma change over time. Additionally, it is often possible to find time-independent solutions to the equations [e.g., Boyd and Sanderson, 2003]. When a plasma system is disturbed, however, it may emit waves in response [Kivelson, 1995b]. This section focuses on the waves that result from the disruption of a plasma system governed by the MHD equations. The purpose of this section is not to give a complete treatment of MHD waves, as this is beyond the scope of the present thesis; rather, the goal is to provide a background for the concepts touched on in the thesis by giving an overview of wave phenomena and how waves can result from an MHD formulation of a plasma system.

One way to analyse the response of a system to a disturbance is to assume the system is initially in equilibrium and introduce a small perturbation. Boyd and Sanderson [2003] consider an ideal MHD plasma which is initially, at time \( t = 0 \), in a static equilibrium. This plasma is perturbed, and we can write the plasma properties as a sum of their equilibrium values and a perturbation value:

\[
\begin{align*}
\rho(r, t) &= \rho_0(r) + \rho_1(r, t) \\
u(r, t) &= u_1(r, t) \\
P(r, t) &= P_0(r) + P_1(r, t) \\
B(r, t) &= B_0(r) + B_1(r, t)
\end{align*}
\]

(1.41)

where the subscripts, 0 and 1, represent the equilibrium and perturbed values respectively, and \( u_0(r) = 0 \). The resulting MHD equations are, ignoring products of perturbations:
\[
\frac{\partial \rho_1}{\partial t} = -u_1 \cdot \nabla \rho_0 - \rho_0 \nabla \cdot u_1
\]
\[
\rho_0 \frac{\partial u_1}{\partial t} = -\nabla P_1 + \frac{1}{\mu_0} (\nabla \times B_0) \times B_1 + \frac{1}{\mu_0} (\nabla \times B_1) \times B_0
\]
\[
\frac{\partial B_1}{\partial t} = \nabla \times (u_1 \times B_0)
\]
\[
\frac{\partial P_1}{\partial t} = -u_1 \cdot P_0 - \gamma P_0 \nabla \cdot u_1
\]
(1.42)

Together with an equilibrium equation:
\[
\mu_0 \nabla P_0 = (\nabla \times B_0) \times B_0
\]
(1.43)

The authors now note that we can obtain equations for the perturbation of the density, magnetic field, and pressure in terms of a displacement vector, \( \xi \):
\[
\xi(r, t) = \int_0^t u_1(r, t') dt'
\]
(1.44)

Since \( u_1(r, t) \) is the only time-dependent variable on the right-hand side of the first, third, and fourth equations of (1.42). Substituting into the second equation of (1.42), we find:
\[
\rho_0 \frac{\partial^2 \xi}{\partial t^2} = F(\xi(r, t))
\]
(1.45)

With:
\[
F(\xi) = \nabla (\xi \cdot \nabla P_0 + \gamma P_0 \nabla \cdot \xi) + \frac{1}{\mu_0} (\nabla \times B_0) \times [\nabla \times (\xi \times B_0)]
+ \frac{1}{\mu_0} [(\nabla \times (\nabla \times (\xi \times B_0))) \times B_0]
\]
(1.46)

Solutions to this equation govern both waves and instabilities that result from a disturbance in the plasma. Plasma instabilities will be discussed in more detail in the next section.
To simplify matters further, Boyd and Sanderson [2003] consider an infinite plasma that is initially static and homogeneous. Thus, in equation (1.46), $\nabla P_0 = 0$, $\nabla \times B_0 = 0$, and since the plasma is infinite we can write the displacement vector using a Fourier analysis in both space and time:

$$\xi(r, t) = \sum_{k, \omega} \xi(k, \omega)e^{-i(k \cdot r - \omega t)}$$  \hspace{1cm} (1.47)

and we have:

$$\rho_0 \omega^2 \xi = k_0 \gamma P_0 (k \cdot \xi) + \frac{1}{\mu_0} \left[ [k \times (k \times (\xi \times B_0))] \times B_0 \right]$$  \hspace{1cm} (1.48)

The solutions to the wave equations are proportional to complex exponentials, dependent on $k \cdot r - \omega t$: waves propagating parallel to $k$ with an angular frequency $\omega$. The phase velocity of these waves is:

$$v_{ph} = \frac{k}{\omega}$$  \hspace{1cm} (1.49)

where $k$ is the wave number. The relationship between $\omega$ and $k$ is the “dispersion relation” for the given wave mode.

Choosing Cartesian axes such that $B_0 = B_0 \hat{z}$ and $k = k_\parallel \hat{y} + k_\perp \hat{z}$, the resulting component equations are:

$$\left( \omega^2 - k_\parallel^2 v_A^2 \right) \xi_x = 0$$  \hspace{1cm} (1.50)

$$\left( \omega^2 - k_\parallel^2 c_s^2 - k_\perp^2 v_A^2 \right) \xi_y - k_\perp k_\parallel c_s^2 \xi_x = 0$$  \hspace{1cm} (1.51)

$$\left( \omega^2 - k_\perp^2 c_s^2 \right) \xi_z - k_\perp k_\parallel c_s^2 \xi_y = 0$$  \hspace{1cm} (1.52)

where $c_s = \sqrt{\frac{n e^2}{\rho}}$ is the adiabatic sound speed (a result of pressure from the electrons in the plasma) and $v_A = \frac{B}{\sqrt{\mu_0 \rho}}$ is the Alfvén velocity. Solving for non-trivial solutions ($\xi \neq 0$), the first equation is decoupled from the other two and this solution leads to the incompressible shear Alfvén wave. Unlike the
other two solutions, this wave-mode only causes field lines to bend, and does not carry changes in plasma pressure and density [Kivelson, 1995b]. The displacement vector is in the $\hat{x}$ direction, perpendicular to both $B_0$ and $k$. The shear Alfvén wave propagates with $v_{ph} = v_A \cos \theta$, where $\theta$ is the angle between $k$ and $B_0$.

The other two modes are the fast and slow magnetosonic modes. In the limit of perpendicular propagation, the fast wave fully combines the compression of the magnetic field and the plasma compression to drive the wave, while the slow wave does not propagate. In the other extreme, for parallel propagation the waves are fully separated into compressional Alfvén and acoustic modes; the latter is driven by fluctuations in gas pressure with the displacement vector along $B_0$, while for the former, the compressibility of the plasma has no effect. In between, the modes are coupled.

The fast-mode waves propagate at a speed of $v_{f_{ms}}$, where:

$$v_{f_{ms}}^2 = \frac{1}{2} \left( c_s^2 + v_A^2 \right) \left[ 1 + \sqrt{1 - \frac{4c_s^2v_A^2 \cos^2 \theta}{(c_s^2 + v_A^2)^2}} \right]$$  \hspace{1cm} (1.53)

So far, we have assumed an Ideal MHD model, which leads to the three types of waves most commonly referenced in the literature. A more complete model, taking into account dissipation (through resistivity, for example), a non-stationary initial equilibrium, or other factors, gives rise to other types of waves, as well as instabilities. Additionally, waves in a realistic plasma are not monochromatic, and the frequency can depend on the wavenumber non-linearly, such that the wave’s properties will change as it propagates, resulting in dispersion [Boyd and Sanderson, 2003]. Thus, in discussing the nature of waves in a plasma, dispersion curves relating the frequency and wavenumber for different solutions to the wave equations are common. An example of such a diagram is given in Figure 1.1.

**Plasma Instabilities in MHD**

Both studies in the thesis involve the kinetic thermalization of an ion distribution on encountering the shock. In Chapter 2, the ions are separated in phase space by the reflection of a fraction from the shock. In Chapter 3,
Figure 1.1: Typical dispersion curves plotted as angular frequency, $\omega$, vs. wavenumber, $k$, for obliquely propagating waves in a warm plasma: whistler (W), ion acoustic (I-A), electrostatic ion cyclotron (ESIC), electromagnetic ion cyclotron (EMIC), fast magnetosonic (FMS), Alfvén (A), slow magnetosonic (SMS). The mark on the horizontal axis denotes unity. From Schwartz [1980].
transmitted ions are thermalized due to the unequal deceleration of different parts of the distribution. In both cases, true thermalization (resulting in a Maxwellian distribution) occurs downstream, with various plasma instabilities proposed as the driving mechanism. In this section, we provide an overview of plasma instabilities and how some of these can arise from the MHD equations.

Stability, in the context of a plasma system, refers to the behaviour of a system in equilibrium when it undergoes small perturbations. If the equilibrium is such that the forces acting in response to the perturbation serve to restore the equilibrium, the system is in a stable equilibrium state. If, however, the system diverges from the original equilibrium state after perturbation, it is unstable. Plasma instabilities are categorized as either macroscopic, pertaining to the spatial displacement of the plasma (where MHD is valid), and microscopic, arising from changes in the velocity distribution function (and therefore requiring kinetic theory rather than MHD).

From a mathematical standpoint, instabilities arise in the MHD equations through the solutions to equation (1.45). Boyd and Sanderson [2003] assume that the displacement can be separated into space and time components, such that:

\[ \xi(r, t) = \xi(r)e^{\omega t} \]  \hspace{1cm} (1.54)

where equation (1.45) becomes:

\[ -\omega^2 \rho_0 \xi(r) = F[\xi(r)] \]  \hspace{1cm} (1.55)

Since \( F \) is linear in \( \xi \), this is an eigenvalue problem where the possible values of \( \omega^2 \) are determined by the boundary conditions; the general solution, then, is the sum over all possible values:

\[ \xi(r, t) = \sum_n \xi_n(r)e^{\omega_n t} \]  \hspace{1cm} (1.56)

\( \xi_n(r) \) is the "normal mode" which corresponds to the "normal frequency", \( \omega_n \). For any normal mode, the eigenvalue \( \omega_n^2 \) is real, and we can see from equation
(1.56) that if $\omega_n^2 > 0$ for all $n$, all the modes are periodic and the general solution oscillates about the equilibrium state. However, if any of the normal frequencies are complex, the normal mode associated with it will grow or decay exponentially and, in the case of exponential growth, the equilibrium is unstable.

For a realistic plasma, such a treatment might only be possible through numerical methods; however, there is a simpler method of determining whether a given equilibrium is stable: the energy principle. The energy principle states that an equilibrium is unstable if the change in potential energy is negative ($\delta W < 0$) for some displacement, $\xi$ [Boyd and Sanderson, 2003].

1.1.5 The Solar Wind as a Collection of Particles: Kinetic Theory

The key assumption of MHD is that the fields and fluids fluctuate similarly in both space and time. However, at a shock this assumption breaks down. As will be explored later, many of the predictions of MHD relating to plasmas are still relevant at shocks, as they are based on the fundamental conservation laws (of mass, momentum, and energy). This allows us to make statements about the relationship between the downstream and upstream fluid parameters. However, since the focus of this thesis is on what happens through and around the shock front on a kinetic scale, we require a different approach.

Rather than treating the particles as a fluid, as in MHD, kinetic theory describes the evolution of a distribution of particles in phase space. One immediate advantage to this approach is that it preserves behaviours that depend on the velocities of the individual particles, rather than only their positions - the fluid variables of MHD, in contrast, are functions of only position and time.

In the extreme, we can define a distribution function which contains information on the exact positions and velocities of all the particles in the plasma:

$$f_N^{ext}(r_1, v_1, \ldots, r_N, v_N, t) = \prod_{i=1}^{N} \delta[r_i - R_i(t)]\delta[v_i - \dot{R}_i(t)] \quad (1.57)$$

where $R_i$ is the location of the $i$th particle at time $t$ and $\delta$ is the delta function (which is infinite at 0 and 0 elsewhere). The function $f_N$ is zero everywhere
except at the point in $6N$-dimensional phase space which corresponds to the locations and velocities of all $N$ particles at time $t$. We can see how this function evolves over time by taking the partial derivative with respect to time [Boyd and Sanderson, 2003]:

$$\frac{\partial f_N^{ex}}{\partial t} = \sum_{i=1}^{N} \left[ \dot{R}_i \frac{\partial f_N^{ex}}{\partial \dot{R}_i} + \ddot{R}_i \frac{\partial f_N^{ex}}{\partial \dot{R}_i} \right]$$

$$= - \sum_{i=1}^{N} \left[ \ddot{R}_i \frac{\partial f_N^{ex}}{\partial \dot{R}_i} + \dot{R}_i \frac{\partial f_N^{ex}}{\partial \dot{v}_i} \right]$$

$$= - \sum_{i=1}^{N} \left[ \dot{v}_i \frac{\partial f_N^{ex}}{\partial \dot{r}_i} + \frac{F_i}{m} \frac{\partial f_N^{ex}}{\partial \dot{v}_i} \right]$$

(1.58)

So far, there is no advantage to using this distribution function as opposed to a multi-body approach, solving the equations of motion for every individual particle. However, it is often appropriate to use a statistical approach, averaging over the possible starting conditions. Defining $f_N$ such that $f_N(r_1, v_1, \ldots, r_N, v_N, t) \pi_{i=1}^{N} dr_i dv_i$ is the probability of the system being in the volume element about $(r_1, v_1, \ldots, r_N, v_N)$ at time $t$, we arrive at the Liouville equation:

$$L_N f_N = 0$$

(1.59)

where:

$$L_N \equiv \frac{\partial}{\partial t} + \sum_{i=1}^{N} \left[ v_i \frac{\partial}{\partial r_i} + \frac{F_i}{m} \frac{\partial}{\partial v_i} \right]$$

(1.60)

is the Liouville operator. The Liouville equation (or Liouville's equation, used interchangeably) is often written in terms of the Hamiltonian, as we will see in Chapter 3.

A further simplification, leading to kinetic theory, is to restrict our distribution function to a 6-dimensional phase space:
\[ f_K(r, v, t) = \sum_{i=1}^{N} \delta[r - r_i(t)] \delta[v - v_i(t)] \]  

(1.61)

where the subscript \( i \) represents the individual particles. This is called the Klimontovich distribution function [Boyd and Sanderson, 2003], and, just as before, we can obtain a smoother distribution function by averaging over a volume element:

\[ f(r, v, t) = \frac{1}{\Delta r \Delta v} \int_{\Delta r} \int_{\Delta v} df_K \]

\[ = \frac{N(r, v, t)}{\Delta r \Delta v} \]  

(1.62)

Here, we assume that the volume element is large enough to contain a statistically significant number of particles, but small enough that the distribution function does not change radically over the scale of the volume element. We can see that \( f \) is simply the number density within a small volume about the point \((r, v)\) at time \( t \). This distribution function is subject to a continuity equation, similar to both the Liouville equation and equation (1.32) in the fluid model except that, as we are now dealing with a function dependent on both position and velocity, there is an additional divergence term. In general, we have:

\[ \frac{\partial f}{\partial t} + \frac{\partial}{\partial r} (rf) + \frac{\partial}{\partial v} (fv) = 0 \]  

(1.63)

where \( a = \frac{F}{m} \) is the acceleration. Here, \( r \) and \( v \) are independent, so \( \nabla_r \cdot v = 0 \) in the second term. In the absence of collisions, we might also assume that \( \nabla_v \cdot a = 0 \) [Goertz and Strangeway, 1995]. We can see that this is a valid assumption for acceleration due to gravity or an electric field (since these forces depend only on position, not the velocity of the particle), as well as a magnetic field (where the force in a given direction depends on the velocity components orthogonal to that direction). Making this assumption results in the kinetic equation:

\[ \frac{\partial f}{\partial t} + v \frac{\partial f}{\partial r} + \frac{F}{m} \frac{\partial f}{\partial v} = 0 \]  

(1.64)

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This is the Collisionless Boltzmann equation, also known as the Vlasov equation due to Vlasov’s work in the case where the force is due to the self-consistent electric field. In the case of collisions, a non-zero term appears on the right-hand side of equation (1.64).

**Jeans’ Theorem**

One important consideration in discussing the various treatments of plasma mechanics is the equivalence of the theories. Jeans’ theorem demonstrates the equivalence of the Collisionless Boltzmann equation to particle orbit theory.

Let the general solution to the equation of motion $ma = F$ be given by:

\[
\begin{align*}
  \mathbf{r} &= \mathbf{r}(c_1, c_2, c_3, c_4, c_5, c_6, t) \\
  \mathbf{v} &= \mathbf{v}(c_1, c_2, c_3, c_4, c_5, c_6, t)
\end{align*}
\]  

(1.65)

where the $c_i$ are constants of integration. Inverting, $c_i = c_i(r, v, t)$, and we can choose the $c_i$ in terms of the initial values of position and velocity. Now, given any function, $f$, of the constants of integration:

\[
\frac{\partial f}{\partial t} + \mathbf{v} \frac{\partial f}{\partial \mathbf{r}} + \frac{F}{m} \frac{\partial f}{\partial \mathbf{v}} = \sum_{i=1}^{6} \frac{\partial f}{\partial c_i} \left( \frac{\partial c_i}{\partial t} + \mathbf{v} \frac{\partial c_i}{\partial \mathbf{r}} + \frac{F}{m} \frac{\partial c_i}{\partial \mathbf{v}} \right)
\]

\[
= \sum_{i=1}^{6} \frac{\partial f}{\partial c_i} \frac{dc_i}{dt}
\]

\[
= 0
\]

(1.66)

since the $c_i$ are constants of motion. Therefore, any arbitrary function of the integrals of motion is a solution to the Collisionless Boltzmann equation.

\footnote{There is some debate over the name for this equation. Henon [1982] suggests that “Collisionless Boltzmann equation” is the most appropriate choice, though “Vlasov equation” is more commonly found in the literature. For the remainder of the present thesis, we will use the two names interchangeably.}

39
Moment Equations and Temperature

Starting from the Liouville equation, it is possible to develop a rigorous collisional kinetic theory analogous to the (collisionless) Boltzmann equation above, with an additional term on the right-hand side representing collisional forces. Additionally, a relationship between the collisional kinetic theory and the Magnetohydrodynamic equations of section 1.1.4 can be established. Since the solar wind plasma is collisionless, we will not dwell on the mathematics behind this connection here (a complete treatment can be found in, e.g., Balescu [1988]). However, we will briefly investigate one aspect of this relationship: the moment equations.

A “moment” in mathematics expresses the expectation value of powers of a given variable. The $k$-th moment about a value $c$ for a variable $x$ with distribution function $f(x)$ is:

$$\mu_k = \int (x - c)^k f(x) \, dx$$  \hfill (1.67)

By definition, we can see that the first moment about 0 is the mean value of $x$, usually denoted simply by $\mu$. For higher order moments, we are generally more interested in “central moments”, $\mu_k$, which are moments about the mean value ($c = \mu$). The second central moment is called the variance:

$$\mu_2 = \int (x - \mu)^2 f(x) \, dx = \sigma^2$$  \hfill (1.68)

where $\sigma$ is the standard deviation, the square root of the variance.

Moment equations are useful in bridging the gap between collisional kinetic theory, which is cast in terms of a distribution function, and the fluid equations of MHD, which require bulk (average) values. Given a function $f(x, v, t)$ for the density distribution in phase space, as in (1.62), we can find the number density at a given point:

$$n(r, t) = \int f(r, v, t) \, dv$$  \hfill (1.69)
by integrating over all possible velocities. In other words, the number density is the “zeroth”-order moment of the distribution \[\text{[Kivelson, 1995a]}\]. Similarly, the mean velocity of an ensemble is:

\[
\mathbf{u}(r, t) = \frac{\int \mathbf{v} f(r, \mathbf{v}, t) \, d\mathbf{v}}{n(r, t)} \tag{1.70}
\]

where the numerator is the first moment in velocity and the number density appears in the denominator as a normalization term.

We can see that the average total kinetic energy of a fluid is proportional to the second moment, since the kinetic energy for a given particle is \(\frac{1}{2}m\mathbf{v}^2\). The second central moment, on the other hand, is the average kinetic energy due to random motion relative to the mean. This forms the statistical basis for the kinetic temperature (for a monatomic particle):

\[
\frac{3}{2}k_B T = \frac{\int \frac{1}{2}m\mathbf{v}^2 f(r, \mathbf{v}, t) \, d\mathbf{v}}{n(r, t)} \tag{1.71}
\]

The pressure is likewise proportional to the second central moment, by the ideal gas law (1.37).

So far, we have not made any assumptions about the nature of the distribution. Strictly speaking, in order to attribute a single temperature (or pressure) to a system, it must be in a state of thermal equilibrium (the velocity distribution must be Maxwellian). In this context, temperature is defined by the flow of heat - given two collections of particles, they are said to have the same temperature if they are in thermal equilibrium with each other (that is, there is no heat exchange). One is said to have a higher temperature if heat flows from it to the other collection. From this definition, an expression for the temperature can be found in terms of the energy and entropy \[\text{[e.g., Atkins, 1998]}\]:

\[
T = \frac{dE}{dS} \tag{1.72}
\]

This equation, together with the Second Law of Thermodynamics (which states that the entropy of a closed system not at equilibrium increases, approaching
maximum entropy at equilibrium), demonstrates why heat flows from high to low temperature. If a system contains two "containers" with different temperatures which are in thermal contact, a change in energy for the hotter container corresponds to a smaller change in entropy than for the cooler container - thus, if heat flows from hot to cold the total entropy increases, while if heat flowed from cold to hot the total entropy would decrease, violating the Second Law.

If we have an anisotropic distribution, we can define different pressures and temperatures for different directions in terms of the variance in velocity in the given direction. In this case, it may be possible for heat to flow between two collections of particles which have the same bulk thermodynamic (absolute) temperature, since the anisotropic distribution is not in thermal equilibrium. This distinction between the thermodynamic and kinetic temperatures will be especially important in Chapter 3, where we consider the temperature anisotropy which develops through a laminar shock.

Just as in MHD, it is possible to study waves in kinetic theory by using a perturbative approach, expressing the time-dependent distribution function as the sum of an equilibrium distribution and a perturbation. Wave equations and dispersion relations analogous to those discussed previously can be found, using the Collisionless Boltzmann and Maxwell's equations in place of the MHD equations. However, the MHD plasma treatment of waves and instabilities depends only on bulk plasma properties, while kinetic theory retains microscopic details of the entire distribution.

1.1.6 Computer Simulation

A full kinetic treatment of a system of many particles, including self-consistent particle-induced fields, is not feasible analytically. Numerical methods are necessary for the study of the kinetic behaviour of a collection of particles and the changes in the field structure as the system evolves.

Treating both species, ions and electrons, kinetically leads to full-particle simulations; however, a restriction on the use of full-particle codes to simulate a charged plasma is the large ratio between the masses of the ions and the electrons. The spatial and time scales appropriate for modelling electrons may be much smaller than the scale of the subject of interest, requiring smaller time
steps in the simulation run to resolve, an especially important consideration in the 1980s given limitations on computational power. One way around this difficulty is to treat the ions and electrons separately. In a hybrid simulation, which can be viewed as a compromise between the fluid equations of MHD and a full kinetic treatment of the plasma, the ions are treated as particles using standard particle-in-cell methods [e.g., Pritchett, 2003], but the electrons are treated as a massless, neutralizing fluid [Winske et al., 2003]. Thus, the charge of the ions is neutralized while allowing for a simulation scale more suitable to resolving ion behaviour, since it is the ions which are key in determining structure and thermalization at collisionless shocks.

The present thesis is concerned with the kinetic behaviour of individual ions encountering a shock with external electromagnetic fields, and ignores any effects due to particle-particle interactions. However, numerical techniques common to hybrid and full-particle simulations are used to supplement the analytical results of Chapter 3, and the results of previous simulation studies are additionally important to our understanding of typical shock conditions and profiles.

The hybrid simulation code of Winske [1985a] uses the difference forms of Maxwell's equations, which can be derived from the differential forms given previously. From Gauss’ Law for Magnetism, equation (1.10):

\[
\nabla \cdot \mathbf{B} = 0
\]

\[
\Rightarrow \mathbf{B} = \nabla \times \mathbf{A}
\]  

(1.73)

for some vector potential, \( \mathbf{A} \). From (1.73) and (1.11), and since the fields are constant in the transverse directions (represented by the subscript \( t \)):

\[
\mathbf{E}_t = -\frac{\partial \mathbf{A}_t}{\partial t}
\]  

(1.74)

From (1.73) and (1.12), again for the transverse components:

\[
\nabla^2 \mathbf{A}_t = -\mu_0 \mathbf{J}_t
\]  

(1.75)
The electron momentum equation is given by:

$$m_e \frac{dV_e}{dt} = -qn_e (E + V_e \times B) - x \frac{\partial P_e}{\partial x} + qn_e \eta \cdot J$$

(1.76)

where the left-hand side is 0 under a massless electron assumption. In this equation, $\eta$ is an anomalous resistive term. The treatment of the electrons as a massless fluid allows for a stable algorithm on the ion kinetic scale, but necessarily ignores any kinetic effects by the electrons and requires ohmic heating.

In the transverse components, the pressure term vanishes, leaving:

$$\eta^{-1} (E + V_e \times B)_t = J_t$$

$$= qn (V_1 - V_e)_t$$

(1.77)

Solving for $V_{et}$, and substituting into (1.75) using (1.73) and (1.74) for the transverse fields gives $A_e$ and $A_{et}$ as functions of $A_x$, $A_{et}$, $A_y$, and $A_{et}$.

Now, given the velocities at half time-steps and the position and fields at even time-steps, the Lorentz force is used to advance the velocities. An implicit formulation is used, substituting $v^N = \frac{1}{2} \left( v^{N+\frac{1}{2}} + v^{N-\frac{1}{2}} \right)$ into

$$\frac{1}{\Delta t} \left( v^{N+\frac{1}{2}} - v^{N-\frac{1}{2}} \right) = \frac{q}{m} \left( E^N + \frac{v^N \times B^N}{2} \right)$$

in order to obtain a stable algorithm.

The positions of the macroparticles representing the ions are advanced (the velocity multiplied by the time-step is added to the position at the previous time-step), and the bulk density and velocities are calculated. Using a system of equations derived from equations (1.75) and (1.77), $A_t$ is obtained, and this leads to $J_t$ (1.75), $B_t$ (1.73), and $E_t$ (1.77). An energy equation is used to find $T_e$, and $E_z$ can then be found, along with $V_{eT}$.

At some point in the course of the research collected in this thesis, the idea of an investigation into a Hamiltonian formulation of the equations used in simulation codes was considered. As a result, a considerable amount of time was spent investigating the details of various full-particle formulations. Further description of various simulation methods and results as well as references to how these codes have been used in the study of shock-related phenomena can be
found in Appendix B. We find that, while hybrid codes include an anomalous resistive heating term, full-particle codes are able to solve Maxwell’s equations in a way that preserves the Hamiltonian nature of the system, including self-consistent resistive heating due to cross-field instabilities.

1.2 The Earth’s Bow Shock

When a fluid encounters an obstacle, it must alter its flow around the obstacle. Typically, the presence of an obstacle in a fluid system can be modelled like any other disturbance. The obstacle perturbs the fluid equilibrium, and this perturbation propagates away from the obstacle as a wave. In this way, information about the obstacle is transmitted to the fluid farther away from the obstacle over time, and the flow of the fluid adjusts accordingly.

The speed at which this information can travel is the “speed of sound” for the fluid. In section 1.1.4, we investigated several types of waves and the corresponding speed of sound for each: the adiabatic sound speed, \( c_a \), for a compressive wave in a neutral fluid; the Alfvén velocity, \( v_A \), for the Alfvén wave; and \( v_{fms} \) and \( v_{sms} \) for the fast-mode and slow-mode magnetosonic waves respectively.

If the obstacle is moving faster relative to the flow than the relevant speed of sound - that is, the flow is supersonic - information cannot propagate ahead of the obstacle fast enough to inform and redirect the flow. Instead, we require a different type of wave: a shock wave. A shock wave travels (relative to the flow) faster than the typical speed of sound in the medium, and additionally causes an abrupt change in the state of the fluid as the flow transitions from supersonic to subsonic. Since the velocity of the flow decreases, the conservation of mass requires that the density increases. Additionally, the energy lost in the slowing of the fluid must be gained elsewhere, in the form of heating and dissipation (entropy increase) [Burgess, 1995].

Because of the solar wind’s high velocity, whenever the solar wind encounters an obstacle, such as a planetary body or a comet, a shock wave may form in front of that obstacle. In front of and around the Earth - generally at a distance of about 12 to 16 Earth radii at the nose [Fairfield, 1971] - is a bow shock, a standing shock wave in space. The precise location of the bow shock depends on
the balance between the solar wind plasma pressure ("ram" pressure) and the magnetic pressure downstream of the shock.

A shock wave caused by, for example, a supersonic jet travelling through the atmosphere changes some of the kinetic energy of the incoming flow into heat through collisions between the air particles within the shock layer. However, the density of the solar wind is too small for the bow shock to be the result of collisions. Because of its low density, the typical collisional mean free path (a measure of how often collisions take place in the medium) is on the order of 1 AU [Parks, 2003]. However, the shock front scale is that of the ion gyroradius [Balikhin et al., 1995], approximately 60km [Schwartz, 1985], while the shock ramp width depends on the wavelength of the phase standing whistler wave, between the ion and electron inertial scales, $\frac{\omega_i}{\omega_{pi}}$ and $\frac{\omega_e}{\omega_{pe}}$ [Mellott, 1985]. As the bow shock is collisionless, other mechanisms must be responsible for the deceleration of the flow.

A key parameter in determining the properties of shocks is the Mach number, a dimensionless ratio between the solar wind velocity, $V_{sw}$, and the speed of the relevant waves in the plasma. The (fast) magnetosonic Mach number, then, is the ratio of the solar wind velocity to the propagation speed of the fast-mode waves ($M_{ms} = \frac{V_{sw}}{V_{fms}}$). The Alfvén Mach number, $M_A$, is often used as a close approximation to $M_{ms}$, as it does not depend on the angle of propagation, $\theta$. Schwartz [1985] characterizes shocks with $M_A \leq 3$ as low Mach number shocks, and from the average solar wind parameters given there we can calculate a typical range of $M_A = 5 - 14$.

Figure 1.2 illustrates the shape of the bow shock, as well as other plasma and magnetic field structures surrounding the Earth. The majority of the solar wind ions are decelerated and deflected by this bow shock so that they flow around the Earth. The solar wind can be responsible, through its effect on the Earth's magnetosphere, for satellite and radio interference through geomagnetic storms, as well as the Aurora Borealis (the "Northern Lights") and their southern counterparts, the Aurora Australis, which are caused by energetic charged ions colliding with molecules in the atmosphere and releasing energy in the form of light.

In this section, we identify the key ideas in our understanding of ion behaviour at collisionless shocks arising from in-situ observations in space, theoretical developments, and computational modelling.
Figure 1.2: Diagram illustrating the regions and boundaries that result from the interaction of the supersonic solar wind with an obstacle, the Earth (and its magnetic field), including the bow shock. From Russell [1987].
1.2.1 Wave Steepening and Shock Formation

In an ordinary fluid, shock waves are formed by wave steepening. For fluids following the adiabatic gas law, \( P \rho^\gamma = \text{constant} \), the speed of sound is proportional to \( \rho^{-\frac{1}{\gamma-1}} \). Because the density of a compressional wave is greater at the peak than elsewhere, the speed of sound at the peak is also greater (for \( \gamma > 1 \)), and the shape of the wave distorts as the peak catches up to the rest of the wave, eventually resulting in a discontinuity (where the flow becomes nonadiabatic) [Parks, 2003]. Compressional waves in an MHD plasma can likewise steepen to form shocks (intermediate waves do not), as first shown by Montgomery [1959] (see Figure 1.3).

Ideal MHD assumes collisions between particles in the medium, whereas the Earth's bow shock (for example) is collisionless. Boyd and Sanderson [2003] note three major differences in the nature of a collisionless shock as compared to a collisional shock. First, whereas at a collisional shock a balance is struck between convective and dissipative effects, the collisionless shock is typically formed through dispersive effects. Second, in a collisional plasma collisions at and near the shock front serve to restore the downstream plasma to an equilibrium Maxwellian distribution; the density, velocity, and temperature change through the shock, but we can relate the conditions downstream to those upstream without regard to the actual structure of the shock. These "jump" conditions are discussed in the next section. In contrast, in a collisionless plasma there is no corresponding mechanism to restore the distribution to a Maxwellian, and anisotropic distributions prevail well into the region downstream of the shock until they are eventually thermalized by other mechanisms, such as plasma instabilities [e.g., Sckopke et al., 1990]. Third, because collisional shocks have a width on the order of the collisional mean free path, particles must undergo a transition from an upstream to downstream state (through collisions) before they can pass through the shock, and the two populations are kept separate physically. At a collisionless shock, one of two alternatives could be responsible for keeping the upstream and downstream plasmas separate: either the magnetic field strength is sufficient such that the Larmor radius is smaller than the width of the shock, or instabilities may lead to turbulent dissipation with a mean free path corresponding to the shock width.

Mellott [1985] describes how dispersion can limit wave steepening and lead to the formation of a shock, as illustrated in Figure 1.4. Long wavelength
Figure 1.3: Illustration of wave steepening. The speed of sound at the peak of the wave (A) is greater than elsewhere (B), and the wave steepens as the peak overtakes the rest of the wave. This results in a wave of "permanent form": a shock. From Parks [2003].
Figure 1.4: Example of two dispersion relation types (left) and the resulting shock structures (right). From Mellott [1985].
perturbations in the plasma steepen as discussed above until reaching a scale length \((k_0\) in the figure) such that the wave becomes dispersive. For \(k > k_0\) (shorter wavelength), the phase velocity decreases (1) or increases (2), and further steepening is prevented as these shorter wavelength waves trail the shock or propagate ahead of the shock respectively. The scale of the shock is then determined by the wavelength which will “phase-stand” with respect to the shock.

Another mechanism for limiting wave steepening in the formation of shocks is that found at “resistive” shocks. As with the dispersive shocks described above, the shock thickness is determined by the dispersive scale lengths. As the angle between the magnetic field and the shock normal approaches 90°, this scale length decreases, and as a result the cross-field current increases to trigger electrostatic turbulence. Effectively, this “anomalous” resistivity takes the place of collisions: particles encountering the shock are affected by changes in the fields, resulting in changes in their velocities, much the same as if they collided with other particles [Burgess, 1995]. The resistivity limits the current, which in turn limits the field gradient and wave steepening [Mellott, 1985].

Collisionless shocks are classified by the presence of turbulence, which is dependent on the upstream conditions (Figure 1.5). Strictly speaking, if there is no turbulence and no collisional dissipation, there is no shock [Boyd and Sanderson, 2003]; however, if the turbulence is weak and on a small scale relative to the shock width such that the field and plasma parameters change coherently through the shock, the shock is called a “laminar shock”. Two previously discussed parameters, the ion plasma beta, \(\beta_i\), and the magnetosonic Mach number, \(M_{ms}\), are key in determining the nature of the shock. Laminar shocks are found in low \(\beta\), low Mach number plasmas. While these shocks are relatively rare in space observations, the lack of large-scale turbulence makes laminar shocks more suitable to analytical study. Throughout the thesis, we will assume a low \(\beta\) plasma, resulting in either a high Mach number quasi-laminar shock (Chapter 2) or a low Mach number laminar shock (Chapter 3).

### 1.2.2 Rankine-Hugoniot Relations

In deriving the MHD equations, we noted that the hydrodynamic equations are forms of the conservation laws - conservation of mass, momentum, and energy.
Figure 1.5: Quasi-perpendicular shock classification vs. $\beta$ and Mach number. The percentage of observed terrestrial bow shocks which fall in each category is given. The dotted line encloses a region within which 90% of solar wind parameters occur, while the two boxes enclose mean parameters for two observational surveys ±1 standard deviation. From Mellott [1985].
In fact, it can also be shown that the induction equation is also a conservation equation, by the frozen flux theorem [Boyd and Sanderson, 2003]. However, a shock in MHD is a discontinuity, and the MHD equations do not apply within the shock, even for collisional plasmas.

To relate the properties of the plasma upstream and downstream of the shock, another statement of these conservation laws comes in the form of the shock jump conditions, or Rankine-Hugoniot relations. We can solve the ideal MHD equations in the form of these relations, with parameters changing in only one-dimension (normal to the shock) and constant in time (steady state), and with the shock assumed to be in an infinite plane [Petrinec and Russell, 1995]:

\[ [\rho v_n] = 0 \] (1.78)

\[ [\rho v_n^2 + P + \frac{B_t^2}{2\mu_0}] = 0 \] (1.79)

\[ [\rho v_n v_t - \frac{B_n}{\mu_0} B_t] = 0 \] (1.80)

\[ \left[ \rho v_n \frac{v^2}{2} + \frac{\gamma}{\gamma - 1} v_n P + v_n \frac{B_t^2}{\mu_0} - \frac{B_n}{\mu_0} (v_t \cdot B_t) \right] = 0 \] (1.81)

\[ [B_n v_t - v_n B_t] = 0 \] (1.82)

\[ [B_n] = 0 \] (1.83)

where the subscripts \( n \) and \( t \) are the normal and transverse components respectively and the bracket notation denotes a change in the quantity from upstream to downstream. These equations express the conservation of mass,
momentum (normal to and transverse to the shock), and energy, as well as the continuity of the tangential electric field and the normal magnetic field (from Maxwell’s equations). Note that there are six equations and six unknowns; thus, for a one-fluid, isotropic, MHD plasma, the Rankine-Hugoniot relations have a unique solution and the downstream conditions are completely determined by the upstream parameters. Petrinec and Russell [1995] show how these equations can be solved for the ratio between the downstream and upstream density (or velocity), \( X \), in terms of the upstream conditions. In general, the resulting equation in \( X \) is quartic, which can be reduced to a cubic by factoring out the trivial non-shock solution, \( X = 1 \) (no change in the plasma parameters from upstream to downstream):

\[
0 = A_1 X^3 + B_1 X^2 + C_1 X + D_1 
\]

\[
A_1 = (1 + \gamma)M_A^6 \cos^6 \alpha_{un} 
\]

\[
B_1 = M_A^4 \cos^4 \alpha_{un} \left[ (1 - \gamma)M_A^4 \cos^2 \alpha_{un} - (\gamma + 2) \cos^2 \theta_{bn} - \gamma(1 + \beta) \right] 
\]

\[
C_1 = M_A^2 \cos^2 \alpha_{un} \left[ (-2 + \gamma + \gamma \cos^2 \theta_{bn})M_A^2 \cos^2 \alpha_{un} + (1 + \gamma + 2\gamma \beta) \cos^2 \theta_{bn} \right] 
\]

\[
D_1 = \cos^2 \theta_{bn} \left[ (1 - \gamma)M_A^2 \cos^2 \alpha_{un} - 3\gamma \cos^2 \theta_{bn} \right] 
\]

where \( \theta_{bn} \) is the angle between the magnetic field and the shock normal, and \( \alpha_{un} \) is the angle between the (upstream) bulk velocity and the shock normal. From this equation, a real root (and therefore the downstream conditions) can be determined in terms of the upstream conditions. However, if another fluid (electrons, for example) is introduced, or if the pressure is anisotropic, additional variables appear and further assumptions must be made to solve the relations uniquely [Burgess, 1995].

The studies in the thesis do not allow for unique solutions to the Rankine-Hugoniot relations, due to non-planar shock geometries in Chapter 2 and anisotropic downstream distributions in Chapter 3, and so we will not dwell on R-H calculations for the shock parameters used. However, it is important to note that the conservation of momentum in particular is important for both specular reflection and Hamiltonian mechanics. We will additionally discuss the validity of the steady state approximation, assumed throughout, in Section 2.4.
1.2.3 Observations at the Earth's Bow Shock

Of obvious importance in both identifying the bow shock and in studying the properties of the solar wind upstream of and through the shock have been observational results from various space missions. Initial missions, beginning with NASA's Pioneer 1 and the Luna series of Soviet missions in the late 1950s (the first to unambiguously detect the solar wind [Gringauz et al., 1960; Shklovsky et al., 1960]), were limited to measurements by single spacecraft, making it difficult to separate spatial and temporal scales. ISEE, launched in 1977 and 1978, was the first multicraft mission to study the bow shock and solar wind conditions, with three spacecraft: two in similar orbits and one kept upstream of the shock to measure solar wind conditions. The more recent Cluster mission (2000) includes four spacecraft, in order to resolve spatial phenomena in three dimensions.

In this section, we will discuss a selection of observations and simulation studies which highlight the distinction between ions that are directly transmitted through the shock into the downstream region and ions which arrive downstream only after initially undergoing reflection from the shock, noting the importance of the angle between the magnetic field and the shock normal, $\theta_{bm}$, in determining the subsequent behaviour of the reflected ions and how this naturally seems to lead to the observed dichotomy between quasi-perpendicular and quasi-parallel shocks. We will also present a brief overview of the theoretical explanations of these observations, which will be expanded on in later chapters.

Reflection and Heating

One of the significant theoretical properties of a collisionless shock is that, above a critical Mach number, $M_c$, resistive heating is no longer sufficient to account for the dissipation that occurs through the shock [Paul et al., 1965; Tidman and Krall, 1971]. Early studies using both laboratory experiments [e.g., Phillips and Robson, 1972] and numerical simulations [e.g., Forslund and Freidberg, 1971] indicated that the additional mechanism responsible for dissipation at supercritical shocks is the reflection of a significant portion of the ions from the shock. Reflection results in a dispersion of the ions in velocity space, and thus an increase in temperature.
Observational results such as those presented in Figure 1.6 [ISEE, from Sckopke et al., 1983] verify these predictions. The first frame shows the unperturbed solar wind, while in the following frames we can see secondary distributions. The first few frames are in good agreement with predicted velocity calculated with the assumption that some of the incident ions are specularly reflected at the shock, though the authors note that there is a discrepancy between the observed and the predicted distributions in the latter frames, perhaps due to an element of non-specular reflection.

Figure 1.7 demonstrates the difference in structure between subcritical and supercritical shocks that results from the degree of ion reflection in the latter. A subcritical shock crossing is sharp, with rapid heating and little noise. In contrast, the magnetic profile at a supercritical crossing exhibits both a foot (as ions travel back upstream after reflection before possibly returning to the shock through gyration about the magnetic field) and overshoot, as well as significant oscillation in the magnetic field strength continuing downstream of the shock.

Sckopke et al. [1983] point out that, strictly speaking, thermalization should result in Maxwellian distributions, but they define an “effective” temperature related to the trace of the pressure tensor (the kinetic temperature discussed in Section 1.1.5). In this way, the authors study the change in the kinetic temperature due to the reflection of a portion of the ions. They find that this dispersion accounts for the ion temperatures observed downstream and predicted by conservation relations with no additional heating required, only some mechanism to redistribute the ions in velocity space (to yield thermodynamic equilibrium). Various plasma instabilities are mentioned in the literature as possibilities for this redistribution [Winske et al., 1987; Gary et al., 1993; McKeen et al., 1992; Dendy and McClements, 1993], and later chapters will briefly discuss those specifically applicable to the studies of the current thesis.

Among the key simulation studies which relate to ion reflection are Leroy et al. [1981, 1982], which shows the existence of a significant reflected ion population at high Mach number shocks, and demonstrates how the reflected ions explain structural features of these shocks, such as the foot, ramp, and overshoot; and Burgess et al. [1989], which investigates the origins of the reflected ion and transmitted ion populations in the incident distribution.
Figure 1.6: ISEE snapshots of the ion distribution through a shock crossing, showing distinct populations of ions in phase space due to reflection. Insets (upper-left) show the relative position with respect to the electron density profile, and contours are of constant phase space density. From Sckopke et al. [1983].
Figure 1.7: Magnetic field profiles at a subcritical crossing (top) and supercritical crossing (bottom). From Gosling and Robson [1985], adapted from Livesey et al. [1984].
Quasi-perpendicular vs. Quasi-parallel

Observations of the bow shock reveal a striking difference in the properties of the shock which correlates to the angle between the magnetic field and the shock normal, $\theta_{bn}$. The quasi-parallel shock front is characterized by a turbulent region upstream of the shock called the ion foreshock (Figure 1.8). Quasi-perpendicular shocks, in contrast, display a relatively sharp transition, with little turbulence upstream of the shock. Fairfield [1974] provides a histogram (Figure 1.9) counting the number of “clean” transitions and “pulsation” (extended) transitions as a function of $\theta_{bn}$. The author notes that abrupt transitions are almost always limited to the quasi-perpendicular range.

One of the reasons for the marked differences in the nature of the bow shock in the quasi-perpendicular regime vs. the quasi-parallel is the differing behaviour of the ions reflected from these regions of the shock. At a quasi-parallel shock, the ions return upstream, resulting in turbulence, whereas at a quasi-perpendicular shock, the ions gyrate to reencounter the shock and eventually pass downstream. Even for low Mach number quasi-parallel shocks, where reflection is not a major contributor to thermalization, low level reflection may be significant in the generation of large-amplitude waves [Thomsen et al., 1993].

We can see why this distinction occurs by considering the guiding centre motion of the ions for various values of $\theta_{bn}$. The motion of the ions upstream (after reflection) can be broken down into three components, assuming constant fields: gyration about the magnetic field lines, constant motion along the magnetic field lines, and a constant $E \times B$ drift velocity. The component parallel to the magnetic field is directed away from the shock and is most significant when the magnetic field is exactly parallel to the shock normal ($\theta_{bn} = 0^\circ$). In contrast, the drift velocity is directed toward the shock and is most significant when the magnetic field is exactly perpendicular to the shock normal ($\theta_{bn} = 90^\circ$). These two components together comprise the guiding centre velocity. For a quasi-parallel shock, then, the guiding centre is away from the shock, and the reflected ions stay upstream, forming the turbulent ion foreshock, while for a quasi-perpendicular shock the guiding centre motion is toward the shock and the ions will reencounter the shock after gyration, gaining energy to overcome the shock potential [Gosling et al., 1982]. The focus of Chapter 2 of the present thesis will be on the ranges of $\theta_{bn}$ for which reflected ions either escape upstream, reencounter the shock only to be reflected again, or reencounter the
Figure 1.8: Diagram showing the structure of the bow shock and ion foreshock. Note the extended foreshock associated with the quasi-parallel section of the shock, where $\theta_{bn} < 45^\circ$. From Schwartz [1985].
Figure 1.9: Histogram of the number of cases of "pulsation" and "clean" shock crossings as a function of the angle between the upstream magnetic field and the shock normal. From Fairfield [1974].
shock with sufficient velocity to pass through the shock and continue downstream.

Collisionless Dissipation: Low Mach Number Shocks

At subcritical shocks, ion reflection is no longer significant for dissipation. ISEE measurements show that only about 1-3% of the ion distribution undergoes reflection when $M_A \approx 2$, as opposed to 15-25% for $M_A = 8 - 12$ [Scopke et al., 1983]. Because of this, the most significant contribution to thermalization is the transmitted ion distribution. Figure 1.10 [Thomsen et al., 1985] shows an observed example (again from ISEE) of the temperature change that the ion and electron distributions experience through a subcritical shock. There are two important features of the ion temperature evolution visible in this figure that will be discussed in Chapter 3. First, the heating is rapid, and is completed by the end of the shock ramp. Second, we can see that the temperature downstream of the shock is anisotropic, as heating occurs preferentially perpendicular to the downstream magnetic field.

Typically, the shock width is small relative to the ion gyroradius, and therefore the observed thermalization is unlikely to be the result of turbulence, which occurs on a longer spatial scale [Giacalone et al., 1994]. Thus, our focus will be on the dissipation arising from changes in the ion distribution caused by changes in the electromagnetic fields within the shock.

We can see qualitatively in Figure 1.11 how this dissipation can result simply from an electrostatic potential jump at the shock [Ellacott and Wilkinson, 2006]. For a given ion, the kinetic energy is $KE = \frac{1}{2}mv^2$. The electrostatic potential decreases the kinetic energy by a fixed amount, so the energy difference between any two ions remains the same. However, because the relationship between the kinetic energy and the velocity of an ion is quadratic, a given change in kinetic energy will not yield the same change in velocity for every ion. As a result, the spread in velocities downstream is greater than the spread of the velocities upstream.

Regarding one of the key features of the temperature evolution mentioned above, that the heating is anisotropic, Gedalin [1996b] finds in an analytical study that the potential jump is insufficient to slow the ions to the velocity given by the Rankine-Hugoniot conservation relations. This causes a gyration of
Figure 1.10: ISEE measurements of the ion density, ion velocity, ion temperature, and electron temperature (top to bottom) for a subcritical shock crossing. In the third and fourth panels, two temperature components are plotted: the temperatures perpendicular and parallel to the magnetic field. The two parallel vertical lines in the centre of the diagrams indicate the extent of the shock ramp. From Thomsen et al. [1985].
Figure 1.11: Diagram illustrating how an increase in the spread of velocities results from an electrostatic potential jump, though the spread in kinetic energy remains unchanged. From Ellacott and Wilkinson [2006].
the distribution about the downstream magnetic field. Since the gyration occurs perpendicular to the magnetic field, we can see how this behaviour contributes to the observed temperature anisotropy, $T_1 > T_||$. Chapter 3 will investigate this aspect of the interaction of the transmitted ions with the shock in greater depth.

1.3 Concluding Remarks

In the previous sections of this chapter, we have provided a general overview of the background information necessary to understand the contributions to knowledge made by the research presented in this thesis. Our investigation concerns two aspects of the behaviour of ions at collisionless shocks.

Chapter 2 concerns the reflection of ions from shocks, as this is a key contributor to the heating and deceleration of the plasma flow at high Mach number collisionless shocks. Previous studies have examined the trajectories of reflected ions assuming the shock to be an infinite plane. A model is developed to describe the trajectories of particles after reflection for a variety of shock surface geometries. Of particular interest are the initial conditions which allow the particle to return to the shock with a greater normal velocity than at first encounter, or to return to the shock at all. Results on the effect of the magnetic field direction and the curvature of the shock are discussed for cylindrical, spherical, and parabolic shock geometries and compared to those for a planar shock. In addition, the effect of varying the velocity of the incoming ions or the velocity of the shock is considered.

Chapter 3 examines the evolution of the ion velocity distribution at a quasi-perpendicular shock under low Mach number conditions, where the contributions of reflected ions to shock thermalization is of secondary importance. A purely Hamiltonian formulation is used, and upstream forms of the invariants of the flow are determined. Various properties of the distribution through the shock are then studied, including the phase volume and shape of shells of constant probability, average trajectories, and the temperature, both analytically and using numerical calculations.

Finally, Chapter 4 summarizes the findings of the previous chapters in the context of future development within these areas of research.
Chapter 2

Specular Ion Reflection at Non-Planar Shocks

2.1 Introduction

An important mechanism for dissipation at collisionless shocks is the reflection of a portion of the ions by the shock [Auer et al., 1971; Paschmann and Sckopke, 1983; Sckopke et al., 1983, 1990]. Reflection separates the incident ions into two groups (directly transmitted and reflected) which occupy different bands in phase space. Figure 2.1 [Gosling and Robson, 1985] shows how reflection affects the spread of velocities. Far upstream, the ions occupy one band in phase space distributed around the bulk solar wind velocity. Through the shock and downstream, however, the ions occupy two or more phase space locations: in addition to the directly transmitted ions, which are slowed as they overcome the shock ramp, the reflected ions may appear in several distinct bands as they gyrate, possibly passing through a particular spatial plane parallel to the shock more than once. The effective increase in kinetic temperature achieved through this dispersion of the ions in velocity space is of the same order as that required by the Rankine-Hugoniot conservation relations across the shock [Sckopke et al., 1983]. Downstream, other processes - such as plasma instabilities - can further randomize the velocities on a finer scale [e.g. Lacombe and Belmont, 1995; Schwartz et al., 1996; Song and Russell, 1997; and references therein]. The ion cyclotron instability is one such proposed mechanism [Gary et al., 1993; McKea

1Some of the early work on cylindrical and spherical shock geometries that appears in this chapter has been published in Planetary and Space Science [Newman et al., 2007].
Figure 2.1: Idealized sketch of (a) the trajectory of an ion reflected from a planar shock and (b) the ion velocity distributions resulting from specular reflection. From Gosling and Robson [1985].
et al., 1992; Dendy and McClements, 1993], and Dendy and McClements [1993] note that ion cyclotron waves are associated with distributions which combine a bi-Maxwellian core (such as the $T_{\perp} > T_{\parallel}$ distribution of directly transmitted ions through the shock) with a gyrotrropic ring (resulting from, e.g., reflection from the bow shock). The authors show that the excitation of the ion cyclotron instability agrees qualitatively with wave data from the AMPTE/IRM mission.

The fraction of ions reflected from the bow shock is dependent on the upstream conditions, primarily the Mach number. For low Mach number shocks, viscosity in the form of ion reflection is not necessary to account for the heating which takes place through the shock. However, as the Mach number increases beyond a "critical" Mach number, the MHD equations no longer have a solution without the inclusion of viscosity. From the Rankine-Hugoniot relations we can see that as the Mach number increases, the ratio between the downstream and upstream temperatures also increases, and we require a larger reflected portion of the ion distribution to account for this thermalization. Paschmann and Sckopke [1983] use the Rankine-Hugoniot relations to predict the percentage of ions that will be reflected for different Mach numbers and values of the plasma beta, as seen in Figure 2.2.

Previous studies have modelled the trajectories of these reflected ions assuming a locally planar shock, as the radius of the shock is much greater than the gyroradius of the ions for typical solar wind parameters at the Earth's bow shock [Gosling et al., 1982; Schwartz et al., 1983]. One area of interest involves reencounters with the shock. After reflection, there are three possible outcomes for an ion: the ion could fail to reencounter the shock; the ion could return to the shock only to reflect again; or the ion could return with increased speed normal to the shock, allowing it to pass through. Which of the three outcomes occurs for a given ion depends primarily on the angle between the magnetic field and the shock normal, $\theta_{bn}$. Assuming that an ion has an incident velocity equal to that of the bulk, the guiding centre motion is away from the shock for quasi-parallel shocks (where $\theta_{bn} < 45^\circ$), and the ion will eventually escape upstream (though for $39.9^\circ < \theta_{bn} < 45^\circ$ the ion will reencounter the shock due to gyration, allowing for further reflection). For quasi-perpendicular shocks, the guiding centre motion is directed downstream and the particle will reencounter the shock with a greater normal velocity, allowing it to overcome the potential barrier [Schwartz et al., 1983].

In this study, we consider the trajectory of ions reflected from cylindrical,
Figure 2.2: Percentage of ions reflected from the Earth's bow shock vs. magnetosonic Mach number of incoming solar wind. The curves correspond to theoretical predictions based on the Rankine Hugoniot relations for ion temperatures corresponding to $\beta = 0.1$ and $\beta = 10$, and assuming the electrons heat by a factor of 2.5 at the shock. Also included for comparison are observational results from ISEE (filled-in symbols) and values from numerical simulations by Leroy et al. [1982] (asterisks). From Paschmann and Skopke [1983].
spherical, and parabolic shocks. The trajectory depends only on the initial velocity, magnetic field orientation, and shock normal at reflection. However, for a curved shock the normal vector depends on the geometry and the position of incidence. Also, while the trajectory of the ion is the same as it would be for a comparable planar shock, the shock front curves away from the ion as it moves transverse to the shock. The size (curvature) of the shock is treated as a free parameter, so that our analysis may be applied to planetary bow shocks of different sizes and we may investigate the importance of the curvature in determining the eventual fate of a reflected ion.

We also restrict our study to the ions. Though the methodology presented could be applied to a study of electron trajectories in constant electromagnetic fields, electrons encountering the electrostatic potential at a shock will be accelerated rather than reflected, due to their negative charge. The effect of shock curvature on the motion of electrons and, specifically, their acceleration by the shock has been the subject of a number of computational and theoretical studies [e.g. Krauss-Varban and Burgess, 1991; Vandas, 1995a,b, 2001].

Additionally, ion-scale ripples observed on the surface of the quasi-perpendicular bow shock [Lowe and Burgess, 2003; Moullard et al., 2006] provide a possible explanation for electron acceleration and the observed electron distributions downstream of the shock [Lowe and Burgess, 2000; Burgess, 2006]. While in reality the shock front is not a smooth “wall” and the fields are affected by changing solar wind conditions and by the density of the reflected population in the shock foot region [Leroy, 1983; Burgess et al., 1989], this study will assume specular reflection from a smooth, curved surface, with constant electromagnetic fields. This allows the motion to be treated analytically, and allows comparison with previous planar shock studies [Gosling et al., 1982; Schwartz et al., 1983; Wilkinson and Schwartz, 1990]. Likewise, while the size and location of a shock in space are affected by variations in solar wind conditions and changes over time, it is assumed for the majority of the chapter that the shock is stationary for a given ion.

2.2 Method

Whereas many previous theoretical studies conduct their analysis of ion trajectories either in the Normal Incidence frame or the de Hoffman-Teller
frame [de Hoffman and Teller, 1950; Schwartz, 1985], we will keep our treatment general by considering arbitrary orientations of the incident velocity and upstream magnetic field. Using the shock rest frame allows us to preserve symmetry for non-planar shocks.

In a specular reflection, the velocity of the particle normal to the shock is reversed. The normal component is:

\[ \mathbf{v}_n = (\mathbf{v}_1 \cdot \hat{n})\hat{n} \] (2.1)

where \( \hat{n} \) is the unit upstream-pointing shock normal vector at the position of reflection and \( \mathbf{v}_1 \) is the incident velocity. The initial \( (t = 0) \) velocity, immediately after reflection, is:

\[ \mathbf{v}_r = \mathbf{v}_1 - 2\mathbf{v}_n \] (2.2)

As we have seen in section 1.1.2, for a charged particle in the presence of a constant electric and magnetic field, only the velocity perpendicular to the magnetic field changes over time, we separate the velocity of the ion after reflection into parallel and perpendicular components. These are:

\[ \mathbf{v}_\parallel = (\mathbf{v}_r \cdot \hat{b})\hat{b} \] (2.3)

\[ \mathbf{v}_\perp = \mathbf{v}_r - \mathbf{v}_\parallel = \mathbf{v}_r - (\mathbf{v}_r \cdot \hat{b})\hat{b} \] (2.4)

We assume a motional electric field upstream: \( \mathbf{E} = -\mathbf{V}_{sw} \times \mathbf{B} \), where \( \mathbf{V}_{sw} \) is the bulk solar wind velocity. The \( \mathbf{E} \times \mathbf{B} \) drift is:
\[ v_d = \frac{|E|}{|B|} \hat{e} \times \hat{b} \]
\[ = \frac{E \times B}{|B|^2} \]
\[ = \frac{(-V_{sw} \times B) \times B}{|B|^2} \]
\[ = (-V_{sw} \times \hat{b}) \times \hat{b} \]
\[ = V_{sw} - (V_{sw} \cdot \hat{b})\hat{b} \]
\[ = V_{sw,\perp} \] \hspace{1cm} (2.5)

where \( V_{sw,\perp} \) is the bulk velocity perpendicular to the magnetic field.

Both the parallel component and the drift are constant. These are combined to give the "guiding centre" velocity of the ion after reflection, \( v_{gc} \).

\[ v_{gc} = v_d + v_\parallel \]
\[ = V_{sw} + (v_r \cdot \hat{b})\hat{b} - (V_{sw} \cdot \hat{b})\hat{b} \] \hspace{1cm} (2.6)

The remaining velocity component varies due to the magnetic force, which causes gyration about the guiding centre. The gyration velocity, \( v_g \), immediately after reflection is:

\[ v_g(0) = v_r - v_{gc} \]
\[ = v_r - (v_r \cdot \hat{b})\hat{b} \] \hspace{1cm} (2.7)

where \( v_r = v_r - V_{sw} \).

Figure 2.3 illustrates the velocity components \((v_i, v_r, v_\parallel, v_d, v_{gc}, \text{and } v_g(0))\) for an arbitrary initial velocity and magnetic field orientation.

In order to find the gyration velocity at time \( t \) after reflection, we need to solve for the constants of integration in equations (1.18) and (1.19). Using \( v_g(0) \) as our initial condition we have:
Figure 2.3: Vector diagram of the velocity components for specular reflection from an arbitrary shock geometry. The $v_\perp$ in the diagram is the drift velocity, $v_d = V_{sw,\perp}$ in the text. The vector $(v_r \cdot \hat{b})\hat{b}$ is the parallel component of velocity after reflection, $v_\parallel$. From Gosling et al. [1982].
$$v_g(0) = C \cos(\alpha)\hat{e} + C \sin(\alpha)\hat{k} \quad (2.8)$$

Now for $t \geq 0$:

$$v_g(t) = C \cos(\Omega_c t + \alpha)\hat{e} + C \sin(\Omega_c t + \alpha)\hat{k}$$
$$= C (\cos(\Omega_c t) \cos(\alpha) - \sin(\Omega_c t) \sin(\alpha))\hat{e}$$
$$+ C (\sin(\Omega_c t) \cos(\alpha) + \cos(\Omega_c t) \sin(\alpha))\hat{k}$$
$$= \cos(\Omega_c t) \left( C \cos(\alpha)\hat{e} + C \sin(\alpha)\hat{k} \right)$$
$$+ \sin(\Omega_c t) \left( C \cos(\alpha)\hat{k} - C \sin(\alpha)\hat{e} \right)$$
$$= \cos(\Omega_c t) v_g(0) - \sin(\Omega_c t) v_g(0) \times \hat{b}$$
$$= \cos(\Omega_c t) v_t - \cos(\Omega_c t) (v_f \cdot \hat{b})\hat{b} - \sin(\Omega_c t) v_f \times \hat{b} \quad (2.9)$$

The velocity of the ion at any time, $t$, is then the sum of the guiding centre motion and the gyration velocity:

$$v(t) = v_{gc} + v_g(t)$$
$$= v_{sw} + \cos(\Omega_c t) v_f$$
$$+ (1 - \cos(\Omega_c t)) (v_f \cdot \hat{b})\hat{b} - \sin(\Omega_c t) v_f \times \hat{b} \quad (2.10)$$

Finally, integrating the velocity gives the position of the ion after reflection:

$$r(t) = r_1 + V_{sw} t + \frac{\sin(\Omega_c t)}{\Omega_c} v_f$$
$$+ \left( t - \frac{\sin(\Omega_c t)}{\Omega_c} \right) (v_f \cdot \hat{b})\hat{b} + \frac{\cos(\Omega_c t) - 1}{\Omega_c} v_f \times \hat{b} \quad (2.11)$$

where $r_1$ is the position of the ion at reflection relative to the origin (which we place at the centre of the shock for the cylindrical and spherical models in this study).

For the purposes of determining whether the ion reencounters the shock and whether it does so with an increased normal velocity, the shock size and the
magnitudes of the bulk ion velocity, magnetic field, ion charge, and ion mass can be reduced to a single dimensionless quantity. By expressing the velocity and the time in units of the incident velocity and inverse gyrofrequency, respectively, we simplify the equations by eliminating $\Omega_i$ and expressing the shock size in terms of the upstream gyroradius:

$$v'(t') = -\hat{x} + \cos(t')v'_f + (1 - \cos(t'))(v'_f \cdot \hat{b})\hat{b} - \sin(t')v'_f \times \hat{b} \quad (2.12)$$

$$r'(t') = r'_i - \hat{x}t' + \sin(t')v'_f + (t' - \sin(t'))(v'_f \cdot \hat{b})\hat{b} + (\cos(t') - 1)v'_f \times \hat{b} \quad (2.13)$$

where $t' = 2\pi$ is the time it takes for the ion to complete one gyroperiod following reflection ($t' = \Omega_i t$), $v'$ is a velocity in units of the bulk ion velocity ($v' = \frac{v}{V_{sw}}$), and $r'$ is a position in units of the convected gyroradius, $\frac{r_i}{\Omega_i} = \frac{V_{sw}m}{qB}$. (For the remainder of the chapter, we will drop the prime notation and simply use $t$, $v$, and $r$ to represent time, velocity, and position respectively in terms of these units.)

For a given initial position, velocity, and magnetic field direction, one can calculate $r(t)$ and $v(t)$ for any $t$. In order to determine the ion's closest approach to the shock, we make repeated use of the method of false position [Weisstein, 2005]. First, we find the time, $t_a$, within the ion's first gyroperiod at which the velocity normal to the shock is at a minimum. Here, the acceleration normal to the shock is zero. The acceleration is found by differentiating equation (2.12):

$$a(t) = -\sin(t)v_f + \sin(t)(v_f \cdot \hat{b})\hat{b} - \cos(t)v_f \times \hat{b} \quad (2.14)$$

The calculation of the acceleration (and velocity) normal to the shock depends on the shock geometry chosen, and will be discussed further in the geometry specific sections to follow.

If the minimum normal velocity is positive (away from the shock), the ion's trajectory is directed away from the shock for all values of $t$, and thus the ion
will never return to the shock. If the minimum normal velocity is negative, we note that both the initial normal velocity and the normal velocity at $t = 2\pi$ are positive, and we can again use the method of false position to find $t_b$ in the range $[0, t_a]$ and $t_c$ in $[t_a, 2\pi]$ when the normal velocity is zero. At $t = t_b$, the ion will be at a maximum distance from the shock (within the first gyroperiod). At $t = t_c$, the ion will make its closest approach to the centre of the shock. If its position at $t_c$ is inside the shock, we know that the ion must have reencountered the shock between $t_b$ and $t_c$. Finally, we find $t_d$ in the range $[t_b, t_c]$ such that the distance between the ion and the shock is 0. We can then determine the normal velocity at $t_d$, when the ion reencounters the shock, and compare it with the initial normal velocity.

Note that the velocities and positions given by equations (2.12) and (2.13) are only correct for $t < t_d$, since the ion will be slowed or reflected again on reencountering the shock. In the present study, we are only concerned with whether the ion reencounters the shock (and its incident velocity, if it does reencounter the shock), and so we make use of the values of the velocity and position functions for $t > t_d$ in order to determine $t_d$ (if it exists). In order to apply this model to a study of multiple reflections (for example), we can use the position and velocity at $t_d$ as the initial position and velocity for a subsequent reflection.

This framework is independent of the shock geometry used, and applies to planar shocks as well as curved. For curved shocks the initial normal vector, $\hat{n}$, is dependent on $r_1$. We now consider the problem of calculating the distance to the shock and the normal velocity at any time after reflection for specific shock geometries.

### 2.2.1 Planar Shock Geometry

For a planar shock, we are only concerned with the $x$ component of position and velocity. The incident normal vector is $\hat{n} = \hat{x}$, and so we have $v_n(t) = v_x(t)$. We let $r_1 = 0$, so that the distance to the shock at $t$ is simply $x(t)$. We will assume that the initial bulk velocity is in the negative $x$-direction ($\hat{v}_{sw} = -\hat{x}$). From these conditions, we could solve numerically equation (2.13) for a time, $t$, such that $x(t) = 0$ for any given magnetic field orientation, and then find the limiting $\theta_{bn}$ such that the equation only has one solution in $t$ (that is, the ion only just
returns to the shock). In the special case that the initial ion velocity is also in the x-direction ($v_1 = -v_{zi} \hat{x}$), however, equation (2.13) simplifies to:

$$x(t) = -t + (1 - v_{zi}) \sin(t) + (1 - v_{zi}) \cos^2(\theta_{bn}) (t - \sin(t)) \quad (2.15)$$

Setting the left-hand side equal to zero yields an equation for the time, $t$, when the ion returns to the shock:

$$t - (1 - v_{zi}) \sin(t) = (1 - v_{zi}) \cos^2(\theta_{bn}) (t - \sin(t)) \Rightarrow \cos^2(\theta_{bn}) = \frac{t - (1 - v_{zi}) \sin(t)}{(1 - v_{zi}) (t - \sin(t))} \quad (2.16)$$

The derivative of the right-hand side is zero when $t = \tan t$; this equation has no closed form solution, but we can find numerically that there is a solution within the first gyroperiod at $t \approx 4.49$. The right-hand side has a maximum at this time. In order for the ion to return to the shock, the left-hand side must be less than or equal to this maximum, which depends on $v_z$. When $v_1 = \tilde{v}_{sw}$ (that is, $v_{zi} = -1$), we find:

$$\cos^2(\theta_{bn}) \leq 0.589 \Rightarrow \theta_{bn} \geq 39.9^\circ \quad (2.17)$$

to three significant digits, in agreement with, e.g., Gosling et al. [1982].

We can also find an analytical solution to the problem of an ion returning with equal or increased normal velocity, again assuming that the initial ion velocity is parallel to the shock normal. In this case, from (2.9) we see that $v_{xg}(\pi) = -v_{xg}(0)$ and, integrating (2.9), we also have $x_g(\pi) = 0$ where $x_g$ is the change in x-position due to the gyration of the ion. Thus, if the guiding centre motion is along the shock ($v_{zc} = 0$), at $t = \pi$ the particle will return to the shock and have exactly the same normal velocity as it did initially. Setting $v_{zc} = 0$, then, we find from equation (2.6) that:

$$1 = (1 - v_{zi}) \cos^2(\theta_{bn}) \quad (2.18)$$
When \( v_l = v_{sw} \), this is true for \( \theta_{in} = 45^\circ \); for more perpendicular shocks, the ion will return with an increased normal velocity, since the guiding centre is toward the shock. This is again in agreement with the literature [Schwartz et al., 1983].

2.2.2 Cylindrical and Spherical Shock Geometries

In order to take advantage of the symmetry of a spherical shock geometry, we place the centre of the shock at the origin. The distance between the ion and the shock after reflection is \( |r(t)| - R \), where \( R = |r_i| \) is the radius of the shock. Since the closest point on the shock to the ion will always lie on the line between the ion and the origin, the unit normal vector at that point is \( \frac{r(t)}{|r(t)|} \). Then:

\[
v_n(t) = \frac{v(t) \cdot r(t)}{|r(t)|}
\]

For a cylindrical geometry, we let the axis of symmetry lie along the \( y \)-axis. The calculation of the distance to the shock and the normal velocity is then the same as above, except the \( y \)-components of the position and velocity are ignored.

In this study, we illustrate our model for typical parameters at the Earth's bow shock, with the interplanetary magnetic field, \( \mathbf{B} \), in the \( xz \)-plane, and the solar wind velocity, \( \mathbf{V}_{sw} \), in the \(-x\) direction. Except where \( R \) is a variable, \( R = 114.55 \). This value corresponds to a chosen set of typical parameters: a proton with an incident speed of 400 km/s, \( |\mathbf{B}| = 5nT \), and a shock radius of 15\( R_e \).

2.2.3 Parabolic Shock Geometry

A parabolic geometry presents an additional challenge compared to a spherical geometry. Because of the lack of radial symmetry, the normal vector cannot be directly calculated by dividing the position vector by its magnitude, making it more difficult to find the distance to the shock at an arbitrary point along the ion's trajectory.

For a parabolic shock, a model from Fuselier [1989] is used, where \( x = R - a(y^2 + z^2) \) with \( R = 14.6R_e \) and \( a = 0.0223R_e^{-1} \) (or, in units of the
convected gyroradius: $R = 111.50$, $a = 0.00292$). At any point on the shock surface, the normal vector can be calculated by taking a gradient:

$$n = \nabla(x + ay^2 + az^2) = \hat{x} + 2ay\hat{y} + 2az\hat{z}$$

(2.20)

Now, for a particle located at $r = (x, y, z)$, there is a corresponding point on the surface, $r_s = (x_s, y_s, z_s)$, such that the shock normal at $r_s$ is parallel to $(r - r_s)$. For the moment, we assume that the particle is in the $xz$-plane (the solution can be easily generalized to three dimensions). From equation (2.20), we write:

$$(z - z_s) = 2az_s(x - x_s)$$

(2.21)

And since $r_s$ lies on the shock, $x_s = R - az_s^2$. Substituting for $x_s$ in the previous equation and dividing by the leading coefficient gives:

$$z_s^3 + \frac{1 + 2ax - 2aR}{2a^2}z_s^2 - \frac{z}{2a^2} = 0$$

(2.22)

which is a depressed cubic in $z_s$. Letting $S = \frac{z}{4a^2}$ and $Q = \frac{1 + 2ax - 2aR}{6a^2}$, there is only one real solution as long as the discriminant $Q^3 + S^2$ is positive [Weisstein, 2008]; that real solution is [Stroud and Booth, 2003]:

$$z_s = \sqrt[3]{S + \sqrt{Q^3 + S^2}} + \sqrt[3]{S - \sqrt{Q^3 + S^2}}$$

(2.23)

Outside the shock, where $x > R - az^2$, we have:

$$Q^3 + S^2 = \frac{(1 + 2ax - 2aR)^3}{216a^6} + \frac{z^2}{16a^4} > \frac{2(1 - 2a^2z^2)^3 + 27a^2z^2}{432a^6}$$

(2.24)

Thus, a sufficient condition for a positive discriminant is $a^2z^2 < \frac{1}{2}$, and the corresponding range of $z$ values covers the scope of this study. For the region where the discriminant is negative, there will be three real roots, and it would
be necessary to calculate these to determine which corresponds to the point on
the shock closest to the ion.

Once \( z_s \) is obtained, \( x_s \) is determined from
\[ x_s = R - ax_s^2, \]
and the distance from
the particle to the shock can be calculated, along with the shock normal at \( r_s \),
used in the calculation of the normal velocity. (If \( y \neq 0 \), substitute
\[ w = \sqrt{y^2 + z^2} \text{ and } w_x = \sqrt{y_x^2 + z_x^2} \text{ for } z \text{ and } z_x \text{ in the two dimensional case, and}
\[ y_s = \frac{w_x}{w} \text{ and } z_s = \frac{w_z}{w}. \])

\section*{2.3 Results and Analysis}

We now consider a number of factors which affect whether a specularly reflected
ion will reencounter the shock, and whether it will do so with a greater normal
velocity. With the exception of section 2.3.5, we will make a cold beam
assumption, with \( v_1 = V_{sw} \). For nonzero temperature (that is, a non-negligible
spread of velocities upstream), only that portion of the distribution with the
lowest normal incident velocity would be reflected, and in order to overcome the
potential barrier upon reencounter with the shock (if they return at all) the ions
would require a normal velocity exceeding the minimum normal velocity of the
initially transmitted distribution. A cold beam assumption both simplifies the
calculations and allows us to avoid making assumptions regarding the upstream
distribution and the percentage of ions reflected while focusing on other factors
than the incident velocity. It also enables meaningful comparisons with previous
cold particle trajectory studies [e.g., Gosling et al., 1982; Schwartz et al., 1983;
Sckopke et al., 1983; Wilkinson and Schwartz, 1990].

\subsection*{2.3.1 Curvature}

One effect of the shock curvature is that as the ion gyrates away from the
position of incidence, the shock curves away from it. Thus for certain initial
conditions, an ion might reencounter a plane tangent to the shock at the
position of incidence, but never reencounter the shock itself. Figure 2.4 shows
the trajectory of ions given three different magnetic field orientations, with both
a planar and cylindrical shock given for reference. When \( \theta_{on} \approx 40^\circ \), the ion does
not reencounter the cylindrical shock, even though the \( x \)-coordinate is less than
\( R \) (the radius of the shock) briefly.
Figure 2.4: Ion trajectories over one gyroperiod in the $xz$-plane for various magnetic field orientations: $\theta_{m} = 35^\circ$ (short dash), $40^\circ$ (dotted), $45^\circ$ (dash-dot). Planar (solid) and cylindrical (long dash) shock surfaces are also shown.
Figures 2.5-2.6 show this same effect over a range of curvatures. For both cylindrical and spherical shocks the minimum $\theta_{bn}$ required for each outcome, returning to the shock and returning with an increased normal velocity, was calculated. For large $R$ these values converge to the published planar values [Schwartz et al., 1983] as expected. At $R = 114.55$, the minimum $\theta_{bn}$ differs by about half a degree from the planar values. However, for small $R$, significant discrepancies (several degrees) with the limiting $\theta_{bn}$ values for planar shocks occur. Thus, at Venus, where the solar wind speed and magnetic field strength are similar, the bow shock is an order of magnitude smaller than the Earth's [e.g., Russell, 1985], and we might expect the curvature of the shock to have a significant effect.

Solar wind parameters for other planetary shocks have been observed in various studies [e.g., Slavin and Holzer, 1979, 1981; Slavin et al., 1985]. Some of these parameters are summarized in Table 2.1, along with the corresponding calculated $R$. For the other inner planets, $R$ is much smaller than the value used for Earth's bow shock above, and we can expect the curvature of the shock to have more impact on the behaviour of reflected ions here. Figure 2.7 revisits Figure 2.5, with labels showing the curvatures associated with typical parameters for the different planetary bow shocks as given in Table 2.1.

### 2.3.2 Magnetic Field Orientation

For a spherical shock, ion trajectories were calculated over a range of incidence positions and $\theta_{bx}$ (the angle between the magnetic field and the $x$-axis) values. As Figures 2.8-2.11 show, whether the ion reflects in the quasi-parallel or quasi-perpendicular region of the shock largely determines the outcome for a reflected ion, as it does with a planar shock. For each value of $\theta_{bx}$, the region where the ion does not return appears as an oval centred around the part of the shock where $\theta_{bn} = 0^\circ$ and covering most of the quasi-parallel incidence positions. A ring covers the positions from which an ion will return to the shock after reflection with a lower normal velocity, with $\theta_{bn}$ typically between $40^\circ$ and $45^\circ$, while quasi-perpendicular reflections result in the ion returning with increased normal velocity. The required $\theta_{bn}$ for returning (and for returning with increased normal velocity) varies away from the nose due to the change in $\theta_{zn}$, staying within a degree of the values at the nose except near the edges of the shock region. Due to the asymmetric gyration, the outcomes are not
Figure 2.5: Minimum $\theta_{\text{on}}$ for returning to the shock vs. shock radius (on a logarithmic scale) for spherical (solid) and cylindrical (dashed) shocks.
Figure 2.6: Minimum $\theta_{bn}$ for returning with an increased normal velocity vs. shock radius (on a logarithmic scale) for spherical (solid) and cylindrical (dashed) shocks.
| Planet              | $R_{ss}(R_P)$ | $|B|(nT)$ | $|V_{sw}|(km/s)$ | $R\left(\frac{|V_{sw}|}{\Omega_{sw}}\right)$ |
|--------------------|---------------|-----------|----------------|-----------------------------------------------|
| Mercury (Perihelion) | 1.40          | 46        | 430            | 35.0                                          |
| Mercury (Aphelion)  | 1.40          | 21        | 430            | 16.0                                          |
| Venus              | 1.30          | 10        | 430            | 17.7                                          |
| Earth (Slavin)      | 13.8          | 6.0       | 430            | 118                                           |
| Earth (This Study)  | 15.0          | 5.0       | 400            | 115                                           |
| Mars                | 1.50          | 3.3       | 430            | 3.79                                          |
| Jupiter             | 75.5          | 0.83      | 430            | 999                                           |
| Saturn              | 26.4          | 0.44      | 430            | 158                                           |

Table 2.1: A comparison of parameters at various planetary bow shocks. The value of 430 km/s is given as a typical solar wind velocity in Table 1 of Slavin and Holzer [1981]. Typical values for the magnetic field strength are given in the same table for the inner planets. A scaling factor of $R_o^{-1}(2R_o^{-2} + 2)^2$ is given, where $R_o$ is the radius of the planetary orbit, and we calculate $|B|$ for the outer planets using $R_o$ values from Table 1 of Slavin et al. [1985]. $R_{ss}$, the shock stand-off distance (the distance from the centre of the planet to the nose of the shock), is calculated from observations tabulated in Slavin and Holzer [1979, 1981]; Slavin et al. [1985]. From these parameters, we calculate $R$, the radius of the shock in units of the convected gyroradius.
Figure 2.7: Revisiting Figure 2.5. Minimum $\theta_{bn}$ for returning to the shock vs. shock radius (on a logarithmic scale) for spherical (solid) and cylindrical (dashed) shocks. $R$ values corresponding to typical planetary bow shock parameters are marked.
Figure 2.8: The outcome of an ion reflecting from a range of positions of incidence (shown as a projection onto the $zy$-plane). The boundaries are for returning to the shock (dash) and returning with the same normal velocity (solid). Within the inner region, the ion does not reencounter the shock; in the middle ring, it reencounters the shock with a slower normal velocity; in the outer region, it reencounters the shock with a faster normal velocity. $\theta_{bz} = 0^\circ$. 
Figure 2.9: As in Figure 2.8, but with $\theta_x = 30^\circ$. 
Figure 2.10: As in Figure 2.8, but with $\theta_{\text{tot}} = 60^\circ$. 
Figure 2.11: As in Figure 2.8, but with $\theta_{bcx} = 90^\circ$. The quasi-parallel regions are now on the left and right sides of the figure. Outside the leftmost and rightmost lines, a reflecting ion will fail to reencounter the shock, while between the two inner lines, a reflected ion will return with a greater normal velocity.
symmetrical with respect to the $y$ coordinate unless the magnetic field is parallel or anti-parallel to the $x$-axis.

### 2.3.3 Shape of the Shock

Figure 2.12 shows the effect of the shape of the shock on the reflection outcome, comparing a parabolic and spherical shock geometry. The shape of this plot is due primarily to the fact that the curvature of a parabolic shock decreases away from the nose, with some skewing due to the change in the orientation of the incident velocity relative to the shock normal. Rather than comparing the parabolic results to those from a fixed spherical geometry, the dashed curve plots results for a spherical shock corresponding to the radius of curvature and $\theta_{zn}$ (the angle between the shock normal and the $x$-axis) of the parabolic shock at that value of $z$. This allows us to focus on changes due to the shape alone. There is little difference between the resulting curves, suggesting that the specific shape is not of direct importance; rather, it is the curvature (relative to the ion gyroradius) and angle of incidence at reflection that determine the variation of $\theta_{bn}$ from the results at a planar shock, and these factors are determined by the shock geometry and the position of incidence.

### 2.3.4 Moving Shock

The bow shock itself is not stationary. Typically, the shock has a velocity in the range of 10-30 km/s [Fairfield and Feldman, 1975]; however, some observations of the shock report velocities over 100 km/s [e.g. Greenstadt et al., 1975; Russell et al., 1982]. In order to attempt to quantify the effect of a moving shock on ion reflection, we consider ions reflecting from the nose of a spherical shock which expands or contracts at a constant speed (with $|V_{shock}| \leq \frac{1}{4}V_{sw}$, corresponding to a range of -100 km/s to +100 km/s for our parameters).

Figure 2.13 shows these results. Perhaps counter-intuitively, a larger $\theta_{bn}$ is required for either outcome as the shock moves away from the centre (that is, toward the Sun) - it is more difficult for an ion to return to a shock that is moving toward it. This is explained by noting that in the shock rest frame, the ion has a increased initial normal velocity. Because of this, the ion's gyroradius after reflection will be larger and the ion will travel further from the nose of the...
Figure 2.12: Minimum $\theta_{bn}$ for returning to the shock vs. $z$ for a parabolic shock (solid). The point of incidence is restricted to the $xz$-plane. The parabolic shock model is $x = R - a(y^2 + z^2)$ with $R = 111.50$, $a = 0.00292$. For comparison, the minimum $\theta_{bn}$ was also calculated for a corresponding spherical shock (dash) with the same radius of curvature and $\theta_{zn}$ at the point of incidence.
Figure 2.13: Minimum $\theta_{bn}$ for returning to the shock (solid) and returning with an increased normal velocity (dash) vs. shock velocity.
shock, and the shock’s curvature becomes more significant, both in determining whether the ion returns (as the shock curves away from the tangent plane at reflection, away from the nose) and whether the ion’s normal velocity is increased (as the orientation of the shock normal changes). The magnitude of the effect is small, less than half a degree over the range studied.

2.3.5 Incident Velocity

Until now, we have assumed that the initial distribution is a cold beam of ions (negligible temperature). If we instead assume a Maxwellian distribution with an initial temperature of $T_u$, the distribution has a standard deviation about the mean of $\sqrt{\frac{kT_u}{m}}$ in each component of velocity, where $k$ is Boltzmann’s constant. For $T_u = 10^5$K, used in Chapter 3 as a typical “low temperature” value [see also, Sckopke et al., 1983], one standard deviation in a particular direction is about 12% of the bulk velocity. (Chapter 3 will investigate the evolution of an initially Maxwellian distribution through the shock, and we will present a more detailed treatment of the distribution function there.)

For a zero-width shock, the electrostatic potential jump has the effect of instantaneously decreasing the velocity of the transmitted ions in the direction normal to the shock. In this simplified scenario, then, the reflected ions are those ions which do not have some minimum normal velocity sufficient to overcome the shock potential. After reflection, in order for a given ion to pass through the shock upon reencountering the shock it must not only have a normal velocity greater than its own initial normal incident velocity, it must also have a normal velocity at least equal to that of the minimum of the initially transmitted ions.

McKean et al. [1993] note in their investigation into the upstream distribution source of reflected ions at quasi-parallel shocks that the phase space origin and the quantity of ions reflected depends on the field structure of the shock upon reflection, in particular the electric field normal to the shock, $E_x$, and the noncoplanar magnetic field, $B_y$. However, the impact of these fields on the trajectory of the ions occurs within the shock ramp, whereas we are assuming specular reflections from a shock of negligible width. Thus, for the simple treatment here, we will continue with the assumptions held through the rest of the chapter, and assume that the electric field is along the $y$ axis (by $E = -V_{sw} \times B$) and that the magnetic field lies in the $xz$-plane.
Figures 2.14-2.16 show the effect of a deviation in the initial velocity of the ion (relative to the bulk velocity) in the $y$, $z$, and $x$ directions respectively, for a spherical shock. The effects of a change in $v_y$ or $v_z$ are largely due to the effect on the angle between the magnetic field and the velocity immediately after reflection. Thus, a deviation in $v_y$ has almost no effect on the required $\theta_{bn}$, while deviation in $v_z$ has a larger effect, since the magnetic field is confined to the $xz$-plane. Even in the $z$ direction, though, the difference in $\theta_{bn}$ is only about half a degree over the range studied. For low temperatures, we would expect that the deviation in the velocity perpendicular to the shock normal would have little effect on the outcome of a specular reflection.

Likewise, a change in $v_x$ has only a small effect on whether an ion will reencounter the shock and whether it will return with an increased normal velocity; these results in Figure 2.16 are comparable to those given in Figure 2.13, where a moving shock results in an effective increase in the incident normal velocity. However, deviation in $v_x$ does have a pronounced effect on whether the ion will be able to overcome the shock potential. If we assume, for the sake of argument, that the minimum normal velocity required to pass through the shock is the bulk velocity (that is, 50% of the ions are reflected initially), an ion initially encountering the shock with a velocity 25% slower than the bulk would need a magnetic field orientation of $\theta_{bn} > 53^\circ$ in order to have the same or greater normal velocity as the bulk on returning to the shock, a difference of about $7^\circ$ compared to those ions initially encountering the shock with a normal velocity only just slower than the bulk velocity.

The overall effect of the deviation in velocity is more complicated, and depends on all three components together [Burgess et al., 1989] and on the detailed structure of the fields at the shock [e.g., Leroy, 1983], but this simple treatment demonstrates the importance of the initial normal velocity of the individual ions in determining what happens to them after reflection.

### 2.4 Summary and Conclusions

A framework for the study of the trajectories of specularly reflected ions from a curved, collisionless shock has been constructed. The investigation focuses on the factors which determine whether a reflected ion will return to the shock after gyration about the magnetic field and, if so, whether the ion will exhibit
Figure 2.14: Minimum $\theta_{bn}$ for returning to a spherical shock (solid) and returning with an increased normal velocity (dash) vs. deviation in $\delta v_y$ from the bulk velocity.
Figure 2.15: As in Figure 2.14, but with $\delta v_z$. 
Figure 2.16: Minimum $\theta_{\text{on}}$ for returning to a spherical shock (solid), returning with an increased normal velocity (long dash), returning with a normal velocity greater than the bulk velocity (short dash), and returning with a normal velocity at least 87.5% of the bulk velocity (dotted) vs. deviation in $v_x$ from the bulk velocity. The incoming solar wind velocity is in the $-x$ direction, so a negative $\delta v_x$ (left) corresponds to an increased incident normal velocity.
an increased velocity normal to the shock on its return. It was found that the primary factor in these outcomes is the magnetic field orientation relative to the shock normal, $\theta_{bn}$. In the quasi-parallel range ($\theta_{bn}$ near 0°), particles tend to escape from the shock after reflection, while in the quasi-perpendicular range ($\theta_{bn}$ near 90°) particles return with a greater normal velocity. In between, around the range $40^\circ < \theta_{bn} < 45^\circ$, ions may return to the shock after gyration but have a lower normal velocity.

The curvature of the shock may also be significant for the bow shocks of Mercury, Venus, and Mars, while the bow shocks of Earth and the outer planets are large enough relative to the ion gyroradius that the curvature of these shocks is of less importance. Different shock geometries have also been considered, including cylindrical, spherical, and parabolic. The shape of the shock is of negligible significance in comparison to the local curvature and magnetic field orientation at incidence, though the global shape determines these two parameters. Also considered is the effect of varying the incident velocity and the velocity of the shock; of these, the deviation in $v_x$ from the bulk is important for higher temperatures, as ions in the tail of the distribution must not only increase their normal velocity to pass through on reencounter with the shock, but must achieve a minimum normal velocity as required to overcome the shock potential.

The primary focus of this study has been the effect of the curvature of the shock under certain ideal conditions. Future work may involve a closer look at some of the approximations made here, in order to determine the effect on the results of a warm plasma, non-specular reflection, or an inhomogeneous magnetic field in the foot region.

For a "quasi-stationary" shock, fluctuations in the shock location, potential jump, and field strengths occur slowly, over many ion gyroperiods. Since the scale of interest in this study is shorter than one gyroperiod, we can approximate the actual shock with a steady state shock solution and constant upstream fields (or, as in Section 2.3.4, we can assume the shock moves at a constant non-zero velocity). Minor spatial variations in the strength of the magnetic field may be ignored, as the invariance of the magnetic moment implies that the transverse momentum is conserved. Ultimately, we are concerned with the velocity of the ion if and when it reencounters the shock, and here the strength of the magnetic field is comparable to the field strength acting on the incident ion.
2.4.1 Future Work: Self-reformation and Shock Ripples

We now also consider a phenomenon encountered in shock simulations which may require a more sophisticated model of the shock than the approaches used above, where the shock is not quasi-stationary. The term "shock self-reformation" was first coined in Burgess [1989] for the process by which a new shock front periodically appears upstream of the old front. Shock reformation is in fact a consequence of ion reflection [Scholer and Burgess, 2007]. For $\theta_{bn}$ in excess of about 80°, reflected ions initially accumulate in the foot region in front of the shock, and if the fraction of reflected ions is sufficient, the gradual potential increase in the foot region becomes a new shock front. Since the trajectories of these ions after reflection are characterized by gyration about the magnetic field, the process of shock self-reformation occurs on the time and spatial scales of the ion cyclotron motion (the gyroperiod and gyroradius), as illustrated in Figure 2.17. (Lembege and Savoini [2002] additionally suggest non-uniformity in the shock front due to shock rippling, though this occurs on the electron scale and should not affect the results for the much larger ions.)

For lower values of $\theta_{bn}$, the whistler wave in the foot region is involved in shock reformation, as the amplitude of the whistler grows, leading to vortices in the incoming ions and reflected (gyrating) ions in velocity space and eventual phase mixing; the shock reforms at the upstream edge of the non-linear whistler ("whistler-induced reformation") [Scholer and Burgess, 2007].

The limitations of current space observations to a small number of spacecraft makes the detection of shock reformation at a physical shock difficult. Various hybrid and full-particle simulation studies have observed shock reformation [e.g., Biskamp and Welter, 1972; Quest, 1985; Burgess, 1989; Lembege and Savoini, 1992; Shimada and Hoehino, 2000], and efforts have been made to determine the necessary conditions for self-reformation to occur, as opposed to a steady state solution. The results of Lembege and Savoini [1992] show that self-reformation occurs above a critical angle, which is around $\theta_{bn} = 62°$.

However, this critical angle is dependent on the conditions of the simulation [Lembege and Savoini, 2002]; for example, the previous study of Forslund et al. [1984] considers a shock at $\theta_{bn} = 78.7°$, under different conditions, and the authors do not mention self-reformation in their results.

While many of these simulations studies use unrealistic values for the ion/electron mass ratio or the plasma frequency to cyclotron frequency ratio,
Figure 2.17: Simulation example of shock reformation. Velocity vs. position for solar wind protons (lower panel) and pickup protons (upper panel) at intervals of 40% of the ion gyroperiod. From Lee et al. [2005b].
Scholer et al. [2003] demonstrates that the observed reformation is not an artifact of the artificial ratios used, as the ion dynamics are unaffected by the foot instabilities, where differences due to these ratios may be found [Lee et al., 2005b].

Hada et al. [2003] approaches the problem of determining the requirements for a non-stationary shock by setting the fraction of ions reflected from the shock as a free parameter, and attempting to find a steady state solution. The authors find that if this fraction is above a critical value, no steady state solution exists, and therefore shock self-reformation must occur. The critical value increases with increasing Mach number, but decreases with increasing ion temperature, suggesting that self-reformation is a high $\beta$ phenomena. In apparent contradiction to this result, Hellinger et al. [2002] find that nonstationary shocks occur for both cold and high Mach number plasmas. Their study uses a one-dimensional hybrid code, and they conclude that this code isn't suitable for the study of self-reformation. However, more recent studies, such as those by Scholer et al. [2003] and Yuan et al. [2009], also find that shock reformation is a low $\beta$ phenomenon.

Similarly to shock reformation, ion-scale ripples mentioned in Section 2.1, which occur for the high Mach number, quasi-perpendicular shocks under examination in this chapter, affect the orientation and strength of the magnetic field and potential ramp. Both reformation and shock ripples challenge some of the key assumptions of the present and previous studies. Self-reformation results in a shock front location which is neither fixed nor moving at a constant velocity. Instead, the location of the shock front is periodically discontinuous. Additionally, the formation of the new shock front is not instantaneous, but rather a gradual increase in potential. Because of this, the assumption that the ion must overcome the same shock potential on reencountering the shock front as that which reflected it initially may be flawed; likewise, even in the absence of reformation, ripples in the stationary shock front may result in fields which fluctuate significantly in the shock foot region. (Lee et al. [2005a] suggest that the trajectory of the ion itself should not be affected greatly. Energization of the ion is associated with the upstream fields, while the shock ramp itself simply plays a role in reflecting the ions; whatever the strength of the potential, the specular assumption made should remain valid.)

Under the conditions necessary for self-reformation, the time it takes for a reflected ion to reencounter the shock after reflection is a small fraction of one
gyroperiod, while shock reformation occurs on the time scale of one gyroperiod. Additionally, the distance between the original shock front and the newly forming front scales with the distance traveled upstream by the reflected ions - depending on the angle of incidence, a given ion may never reach the new shock front before its gyration carries it back toward the original front. These factors lead us to expect that the newly formed shock front will affect only a small fraction of the reflected ion population, insofar as determining whether they escape upstream or reencounter the (original) shock front. Clearly, then, the effect that shock reformation has on the magnetic field and the potential between the two shock fronts is key in discussing the effect of self-reformation on the reflected ion population.

Because of this, future research on specular reflection at the bow shock for curved (and planar) shock geometries might focus on the effect of non-steady shocks. A rigorous study of ion reflection during a shock reformation event may require full-particle simulation in order to self-consistently model the field and potential in the region between the old and reforming shock fronts. A time-dependent shock potential may make the analytical treatment of the ion trajectory impractical, and therefore the ion’s path would be calculated numerically. As an alternative to a self-consistent full-particle or hybrid simulation, a shock potential model introducing periodic ripples and/or shock reformation, may make the numerical methods applied in Chapter 3 suitable for studying the problem of whether reflected ions are able to overcome the shock potential after an initial reflection, using test particle trajectories over a range of starting conditions (magnetic field orientation and initial ion velocity).
Chapter 3

Transmitted Ion Distributions at Quasi-perpendicular Low Mach Number Shocks

3.1 Introduction

We now turn our attention to thermalization due to transmitted rather than reflected ions. We have seen that for high Mach number shocks, reflection plays a key role in thermalization, with a broad-scale separation of the reflected and transmitted distributions in phase space (followed by finer-scale thermalization downstream through other mechanisms). In contrast, low Mach number shocks show a very low density of reflected ions [e.g.: Thomsen et al., 1985; Greenstadt and Mellott, 1987; Mellott and Livesey, 1987; Sckopke et al., 1990]. Because of this, the dissipation of the incident ions that are directly transmitted through the shock is the biggest contributor to the overall ion thermalization at these shocks.

While low Mach number, low plasma beta (equivalently, low temperature relative to the strength of the magnetic field) conditions are rare at the Earth’s bow shock (Figure 1.5), the scarcity of reflected ions results in a shock transition which is largely free of turbulence [Sagdeev, 1966], without the foot and overshoot found in higher Mach number shocks where reflected ions are

\[1\] The main results of this chapter have been published in Journal of Geophysical Research [Newman et al., 2011].
more prominent [e.g., Russell and Greenstadt, 1979; Leroy et al., 1982]. These "ideal" conditions are the reason why, in spite of their relative rarity, these shocks have attracted much interest from researchers seeking to ascertain fundamental properties of collisionless shocks in the absence of turbulence.

Measurements in space have shown that at low Mach number quasi-perpendicular shocks the heating of the transmitted ions can be completed by the end of the shock ramp (see, for example, Figure 1.6), and the distribution downstream exhibits a $T_\perp > T_\parallel$ anisotropy; that is, there is a preference for heating in the direction perpendicular to the magnetic field [Thomsen et al., 1985; Winske et al., 1986; Sckopke et al., 1990]. While Thomsen et al. [1985] consider plasma instabilities (in particular, a modified two-stream instability) as possible heating mechanisms, simulations and theoretical considerations [e.g., Wilkinson, 1991; Gedalin, 1996b, 1997; Ofman et al., 2009] suggest that these distinctive heating features arise instead from the kinetic behavior of the ions in the ramp and beyond. Recent observations of low Mach number, low $\beta$ shocks by Venus Express provide direct evidence of downstream distributions forming as a result of ion gyration and collisionless kinematic relaxation in the absence of significant levels of wave-particle activity [Balikhin et al., 2008].

A number of theoretical explanations for the heating of the directly transmitted ions at low Mach number quasi-perpendicular shocks have been suggested. The earliest of these, by Lee et al. [1986], proposes that, in the de Hoffman-Teller frame [de Hoffman and Teller, 1950], where the (infinitesimally thin) shock is at rest and the flow lines up with the magnetic field upstream (and downstream) of the shock, the ion distribution immediately downstream of the shock is still aligned with the upstream field, such that some of the incident kinetic energy is dissipated in the form of gyration about the downstream field. The implication of this suggestion is that the distribution is "bunched" near the shock, with thermalization occurring gradually, as opposed to the rapid heating often observed [Winske et al., 1986]. Nevertheless, this model is noteworthy for suggesting the importance of the nonadiabatic (in the sense that the magnetic moment is not conserved) motion of the ions through the shock.

Gedalin [1996b] uses a perturbative approach to model the passage of the transmitted ions through an exactly perpendicular shock ($\theta_{bn} = 90^\circ$). Assuming the ion thermal energy to be much smaller than the kinetic energy this author finds that the heating is due to insufficient and inhomogeneous deceleration of the distribution by the cross-shock potential. Additionally, the potential is
unable to decelerate the ions to the downstream velocity required by the Rankine-Hugoniot relations, and this results in a gyration of the distribution perpendicular to the magnetic field and, consequently, the observed anisotropy. The deceleration of the ions depends nonlinearly on the initial velocity leading to a dispersion of the distribution through the shock. In a subsequent study, Gedalin [1997] generalizes this analysis for the case of oblique low Mach number shocks. Assuming a narrow ramp, low $\beta$ conditions, and an incident Maxwellian ion distribution, approximate expressions are derived for the pressure tensor inside the ramp. An important result highlighted in this study is that, as the drift velocity in the shock normal direction depends on the peculiar velocity of the ions, gradual collisionless gyrophase mixing ensues in the downstream region of oblique shocks. The differential deceleration of the ions in the ramp is confirmed by numerical simulation in Balikhin and Wilkinson [1996], where heating is investigated using the “Local Divergence Rate” (measuring the divergence in trajectories which are initially close in phase space).

Lee and Wu [2000] examine the heating of ions by fast shock waves in the solar corona using a model based on that of Lee et al. [1986]. Assuming a thin shock ramp, the heating is found to increase with increasing mass/charge ion ratios and to depend sensitively on the electrostatic potential at the shock, a result consistent with Gedalin [1997] and Gedalin and Balikhin [2004]. Simulations of a low-Mach number low plasma beta quasi-perpendicular ($\theta_{bn} = 80^\circ$) shock yield a proton temperature anisotropy across the shock of $T_{\perp}/T_{\parallel} \sim 3.5$ [Lee and Wu, 2000].

Ellacott and Wilkinson [2003] (hereafter referred to as EW03) consider the evolution of the ion distribution in phase space for low Mach number, exactly perpendicular shocks from the point of view of statistical mechanics. Because the magnetic field is perpendicular to the shock, the motion of the ions in the direction of the magnetic field ($z$) can be ignored, leaving a two-dimensional system. It is this paper that forms the basis of most of the work in this chapter, as we generalize some of the results to quasi-perpendicular shocks.

In EW03, the authors examine the equations of motion in a Lagrangian/Hamiltonian form and use Liouville’s equation, arguing that the classical form of the phase density distribution based on the Hamiltonian, $H$, can lead to neither an increase in temperature nor a temperature anisotropy downstream of the shock. The authors note that the system is not ergodic, and that the Hamiltonian, is not the correct solution since it depends on the
position variable $y$, whereas the distribution should not. Thus, they seek another solution to the Liouville equation, with the distribution taking the form $f = \exp -\beta A^2$. Here, $A^2$ is a solution of the Liouville equation independent of the temperature (and is equal to the gyroradius, $\rho_u$, far upstream of the shock; this $A$ is not to be confused with $A$, the vector potential). Like $\mathcal{H}$, $A^2$ is an invariant of the flow but, unlike $\mathcal{H}$, it depends only on $x$ (position normal to the shock) and the upstream velocity and not on the other position coordinates (such that $f$ meets a Maxwellian boundary condition far upstream).

In this distribution contours of equal phase space probability do not correspond to contours of equal energy and EW03 argue that it is this property of the distribution that makes heating and temperature anisotropy possible. Upstream, the phase shells corresponding to $A^2 = \text{constant}$ are circles. Through the shock, these shells elongate in the direction of the shock normal ($x$), resulting in an (approximately) elliptical phase shell which rotates about the downstream magnetic field, as observed in different theoretical and computational analyses [Wilkinson, 1991; Gedalin, 1996b, 1997; Zilbersher et al., 1998; Ofman et al., 2009]. Figure 3.1 shows numerically calculated phase shells at different locations through and downstream of the shock, confirming these findings.

Of particular interest is the area of these phase shells. The phase area corresponds to the spread of velocities within the distribution (that is, it is related to the temperature). For moderately low upstream temperatures, the phase space density distribution through the shock adopts a Gaussian form. This enables estimates of the downstream to upstream temperature ratio of between 2 and 4 [consistent with, e.g., Lee and Wu, 2000]. EW03 show that through the shock and downstream of the shock, the phase area ($\Delta_x$) enclosed by a curve of constant $A^2$ is inversely proportional to the modal speed of the ions in the shock normal direction, so that the temperature of the distribution increases through the shock in a manner consistent with the results of Balikhin and Wilkinson [1996]:

$$\lim_{A \to 0} \frac{\Delta_x(A)}{A^2} = \frac{\pi B_u^2 \hat{m} V_u}{\hat{p}_1}$$  \hspace{1cm} (3.1)

where $\hat{m} = \frac{m}{q}$, $V_u$ is the bulk plasma velocity upstream (directed antiparallel to the shock normal), $B_u$ is the magnitude of the upstream magnetic field, and $\hat{p}_1$ is the modal value of the canonical momentum corresponding to motion toward
Figure 3.1: Evolution of a phase shell corresponding to one standard deviation of the ion distribution at $T_u = 10^5 \text{K}$ through a perpendicular shock. From EW03.
the shock \( (p_1 = \hat{m}_1 \hat{z}) \). As the ions are slowed by the shock potential, energy is dissipated in the form of an increased spread of velocities.

In EW06 [Ellacott and Wilkinson, 2006], the authors examine several thermodynamic issues: the thermodynamic temperature, the adiabatic nature of the heating, the entropy, and reversibility. As seen earlier (Figure 1.11), the electrostatic potential jump alone results in an increase in the spread of the velocities upstream. This is because the relationship between the kinetic energy and the velocity of an ion is quadratic; a given change in kinetic energy will not yield the same change in velocity for every ion.

While the flow is nonadiabatic in that the magnetic moment is not invariant (due to the narrowness of the shock as compared with the ion gyroradius), the heating is adiabatic in the thermodynamic sense: \( PV'Y \) is conserved across the shock. Related to the conservation of \( PV'Y \) is the relationship between the internal energy, \( U \), and the temperature, \( T \). For an ideal gas, heating is proportional to change in temperature (as discussed in Chapter 1), and heat is equivalent to the change in internal energy, so:

\[
\Delta U = ncv \Delta T
\]  

(3.2)

Here, we have an apparent contradiction. As seen in Figure 1.11, the potential jump at a shock results in an increased spread of the distribution in phase space, which is equivalent to an increase in (kinetic) temperature. On the other hand, the energy change done by the electric field is reversible with no input in thermal energy and so it would seem we have a change in temperature without a corresponding change in internal energy. In fact, EW06 demonstrates that if the mean and modal velocities of the distribution are the same downstream, there is no change in internal energy. It is only by taking into account the difference between the mean and modal velocities that a change in internal energy is obtained, in agreement with equation (3.2).

The authors also note that the anisotropy of the distribution downstream allows for reversibility. For an isotropic distribution, work may only be obtained via a corresponding change in temperature; if two "reservoirs" of a gas which have the same temperature are brought into contact, there can be no work done (that is, no energy is exchanged). This is not the case if one of the reservoirs is
anisotropic. Because the shock potential jump results in a $T_{\perp} > T_{\parallel}$ anisotropy, the work done on the ions is available as internal reversible work.

In Chapter 2, we observed that specular reflection of a fraction of the ions leads to kinetic heating (and an increase in the kinetic temperature), while “true” thermalization happens downstream, as the ions undergo dissipation as a result of instabilities. Here, we note that thermalization is again a two stage process, even without a separation of the distribution into two (or more) distinct populations in phase space. The potential jump at the shock increases the internal energy and kinetic temperature without a corresponding increase in entropy (that is, this step is isentropic), and the resulting anisotropic distribution is later subject to instabilities which serve to restore the distribution to a maximum entropy Maxwellian distribution (an irreversible process).

As in Chapter 2, we will be focusing on the kinetic heating of the first step, resulting in an anisotropic distribution. With the variety of waves found in plasmas, it is not surprising that there is a corresponding variety in the types of instability found, and several types of instability are suggested as possibilities for downstream thermalization, in addition to the ion cyclotron instability discussed in section 2.1. Two such alternatives for the low Mach number shock ramp - the ion acoustic instability and the two-stream instability - are compared by Winske et al. [1987], who find the heating predicted for the modified two-stream instability (which includes corrections for finite plasma $\beta$) is in good agreement with that observed by ISEE [Thomsen et al., 1985], while noting that the ion acoustic instability needs higher energy for excitation, implying narrower shock widths and greater electric field noise than present in their study's data set. However, both instabilities are able to supply the necessary downstream heating. Regardless of the mechanism, the anisotropy of the ion distribution is an available source of free energy with the potential to excite these instabilities, eventually resulting in the isotropization of the distribution.

In EW07 [Ellacott and Wilkinson, 2007], the authors expand the work of EW03 to quasi-perpendicular shocks (though, unlike EW03, this paper does not undertake an asymptotic analysis of the phase volume). The Hamiltonian used is independent of $z$, but not $y$ (which is related to $\dot{z}$ by $\dot{m} \dot{z} + B_\perp y = \text{constant}$). As in EW03, the required solution to Liouville’s equation is not the Hamiltonian. Because of this, phase shells of constant probability are not shells of constant energy, which leads to the observed anisotropy. The temperature increase is related to the difference in the radii, $R_1$ and $R_2$, of spheres of
constant energy corresponding to the smallest and largest values of $\mathcal{H}$ on the phase shell respectively. These radii are estimated in terms of the magnetic field orientation, $\theta_{bn}$, and thus the dependence of the temperature change on $\theta_{bn}$ is studied. Figure 3.2 gives an example of the phase shell evolution computed in this paper.

Crossings of the Venusian bow shock under very low Mach number and $\beta$ conditions are characterized by stationary oscillations of the downstream magnetic field owing to the gyration of the downstream ion distribution as a whole [Balikhin et al., 2008], consistent with many of the above theoretical and computational results. A subsequent analytical study describing the shock as a discontinuity illustrates the gradual gyrotropization of the ion distribution downstream of the shock through a process of ion gyration and collisionless gyrophase mixing [Ofman et al., 2009]. The analysis shows that one should expect spatially periodic oscillations in the ion pressure and magnetic field downstream of the ramp, and this is backed up by hybrid simulations. The gyrophase mixing is faster for higher upstream thermal speeds, higher magnetic compression across the shock, and smaller $\theta_{bn}$ [Ofman et al., 2009].

In this chapter, we will study the evolution of phase shells of constant probability through and downstream of a low Mach number, low temperature, quasi-perpendicular shock, using a different Hamiltonian formulation than that used in EW07. We generalize some of the results of EW03 to three dimensions, including the calculation of the flow invariants and the phase volume. We derive a general expression for the phase volume through the shock, determining the relationship between the phase volume and the modal trajectory in the small $A$ limit. Finally, we present computational examples, investigating the shape of the phase shells, the phase volume, and the change in temperature downstream. Throughout the chapter, we assume a steady-state shock solution; while shock reformation (discussed further in Section 2.3.6) on the ion gyroperiod time scale has been observed in numerical simulations, it is a high Mach number phenomenon dependent on ion reflection [e.g., Scholer and Burgess, 2007], and should not affect these results.

### 3.1.1 Choice of Hamiltonian

In this section, we describe the equations of motion for an ion in a general system of fixed (steady state) electromagnetic fields in terms of the
Figure 3.2: Phase shell evolution through the shock at an oblique shock, with $\theta_{pn} = 50^\circ$. From EW07.
Hamiltonian, which is a constant function of the generalized position and momentum coordinates. Other studies of particle dynamics under the action of macroscopic electric and magnetic fields include those by Balikhin et al. [1998], who examined the heating of electrons at quasi-perpendicular shocks and McCaffrey et al. [1999] who offer a mathematical description based on differential geometry of the divergence of trajectories in strong gradients of the electromagnetic field. Notationally, we assume that \( x \) is in the direction opposite the shock normal and that the magnetic field lies in the \( xz \)-plane. We also assume that the shock is planar, and therefore that the fields and distributions change only with \( x \). The two core assumptions of one-dimensionality and steady state conditions are at the basis of many theoretical studies of collisionless shock physics [e.g., Scudder, 1995; Jones and Ellison, 1991; Gedalin, 1996b, 1997; EW03]. The validity of these assumptions is supported by numerical simulations [e.g., Goodrich, 1985 and references therein] and by the results of a detailed theoretical/numerical analysis of a low Mach number shock observed in space [Zilbersher et al., 1998].

Hamiltonian mechanics is a reformulation of classical mechanics expressing the physical laws of a system using first-order differential equations (Hamilton's equations) in a \( 2n \)-dimensional phase space [e.g., Goldstein et al., 2002], as opposed to second-order differential equations in an \( n \)-dimensional space (\( F = ma \)). While the resulting equations are equivalent to the equations of Newtonian mechanics, a Hamiltonian formulation allows for an elegant treatment of the invariants (conserved quantities) along trajectories. For a closed system, the Hamiltonian, \( \mathcal{H} \), represents the total energy of the system, which is itself conserved. The Hamiltonian is expressed in terms of \( n \) generalized coordinates, \( x_i \), together with \( n \) corresponding generalized (canonical) momenta, \( p_i \). The equations of motion can then be expressed as:

\[
\dot{x}_i = \frac{\partial \mathcal{H}}{\partial p_i} \tag{3.3}
\]

\[
\dot{p}_i = -\frac{\partial \mathcal{H}}{\partial x_i} \tag{3.4}
\]

(Here, and throughout the chapter, we use a single dot above a quantity to denote the first time derivative of that quantity, and two dots to represent the
second time derivative, in keeping with the literature; thus, $\ddot{r} = \mathbf{v}$ is the velocity and $\ddot{r} = \mathbf{a}$ is the acceleration.)

As in the preceding studies, we must first consider the form of the Hamiltonian to be used, and we have some flexibility in choosing both the coordinate system and the Hamiltonian. In particular, we will consider our options in choosing $\mathbf{A}$, the underlying magnetic potential, for a system with fixed and time independent electric and magnetic fields (as in EW03 and EW07), and then determine the resulting Hamiltonian and generalized momenta.

Starting with the Lorentz Force:

\[
m\ddot{r} = q(\mathbf{E} + \dot{\mathbf{r}} \times \mathbf{B})
= q(-\nabla \psi + \dot{\mathbf{r}} \times (\nabla \times \mathbf{A})) \tag{3.5}
\]

\[
\dot{m}\ddot{r} = -\nabla \psi + \dot{\mathbf{r}} \times (\nabla \times \mathbf{A}) \tag{3.6}
\]

where $\psi$ (the electric potential) and $\mathbf{A}$ depend only on position. In order to derive an expression for the Hamiltonian, we first require the Lagrangian, an analogous quantity in Lagrangian mechanics. In terms of the potentials, $\psi$ and $\mathbf{A}$, the Lagrangian is [Goldstein et al., 2002]:

\[
\mathcal{L} = \frac{1}{2} \dot{m}(\dot{\mathbf{r}} \cdot \dot{\mathbf{r}}) - \psi + \dot{\mathbf{r}} \cdot \mathbf{A} \tag{3.7}
\]

The canonical momenta are defined as partial derivatives of the Lagrangian:

\[
p_i = \frac{\partial \mathcal{L}}{\partial \dot{x}_i}
= \dot{m}\dot{x}_i + A_i \tag{3.8}
\]

And the Hamiltonian is:
\[ \mathcal{H} = \sum_i p_i \dot{x}_i - \mathcal{L} \]
\[ = \frac{1}{2} \dot{\mathbf{r}} \cdot \mathbf{r} + \psi \]
\[ = \frac{1}{2m} \sum_i (p_i - A_i)^2 + \psi \]  
\hspace{1cm} (3.9)

Returning to Hamilton’s equations (3.3) and (3.4) above, we find:

\[ \dot{x}_i = \frac{\partial \mathcal{H}}{\partial p_i} = \frac{p_i - A_i}{m} \]  
\hspace{1cm} (3.10)

in agreement with the definition of the canonical momenta in equation (3.8), and:

\[ \dot{p}_i = -\frac{\partial \mathcal{H}}{\partial x_i} = \frac{1}{m} \sum_j (p_j - A_j) \frac{\partial A_j}{\partial x_i} - \frac{\partial \psi}{\partial x_i} \]  
\hspace{1cm} (3.11)

For a planar shock, we assume all fields vary only in the direction of the shock normal \( (x) \). From \( \nabla \cdot \mathbf{B} = 0 \) (Gauss’s law for magnetism) we have that \( B_x \) is constant. We also assume that the magnetic field orientation is confined to the \( xz \)-plane, so \( B_y = 0 \) (i.e. we neglect the noncoplanar component of the magnetic field [e.g., Goodrich and Scudder, 1984] in the ramp). In terms of the vector potential, the magnetic field is:

\[ \mathbf{B} = \nabla \times \mathbf{A} \]
\[ = \left( \frac{\partial A_3}{\partial y} - \frac{\partial A_2}{\partial z} \right) \hat{i} + \left( \frac{\partial A_1}{\partial z} - \frac{\partial A_3}{\partial x} \right) \hat{j} + \left( \frac{\partial A_2}{\partial x} - \frac{\partial A_1}{\partial y} \right) \hat{k} \]  
\hspace{1cm} (3.12)

We can choose a solution for \( \mathbf{A} \) which is either independent of \( y \) or independent of \( z \). The latter choice is made in EW07. If we instead choose the former:
\[ B_z = -\frac{\partial A_2}{\partial z} \]  
\[ A_2 = -B_z x + \alpha(x) \]  
\[ B_x(x) = \frac{\partial A_2}{\partial x} = \alpha'(x) \]

so \( \alpha(x) = \int B_z \, dx \). Since \( B_y = 0 \), we can choose \( A_1 = A_3 = 0 \).

With \( \psi = \phi(x) - V_u B_{uz} y \), where the terms on the right-hand side are the electrostatic and motional components of the potential, we have for the Hamiltonian:

\[ \mathcal{H} = \frac{1}{2m} \left( p_x^2 + (p_2 + B_x z - \alpha(x))^2 + p_y^2 \right) + \phi(x) - V_u B_{uz} y \]

Thus, our choice of \( A \) results in a Hamiltonian which is linear in \( y \).

### 3.1.2 Liouville’s Equation

We now turn our attention to Liouville’s equation, which governs the evolution of the ion distribution in phase space. The general solution to Liouville’s equation is a function of six invariants of the flow (and thus Liouville’s equation tells us that the actual distribution function is also invariant along trajectories). One of these invariants is the Hamiltonian, which is the total energy of the given particle. Unlike the Hamiltonian, the other invariants we seek do not have an explicit closed-form expression in terms of the phase space variables through the shock. However, we can relate the invariants to the upstream parameters, such that a given set of invariants corresponds to a set of initial conditions (upstream phase space coordinates), or vice versa. In effect, the forms of the invariants found at some point sufficiently far upstream determine the initial
conditions (or, equivalently, are determined by the initial conditions), and the invariant functions are defined such that they have the value of the corresponding upstream constant form along the same trajectory. In the same way, if we can express the upstream distribution function in terms of these upstream invariants, we can express the distribution function through and downstream of the shock in terms of the defined invariants. We can then investigate properties of the distribution using this expression.

As in EW03, we let \( f \) be the steady state particle density distribution in phase space and assume that the upstream distribution takes a Maxwellian form (in which the component velocities are normally distributed about the bulk velocity with a standard deviation \( \sqrt{\frac{kT_u}{m}} \), where \( k \) is Boltzmann's constant and \( T_u \) is the upstream temperature) [see also Gedalin, 1997]. In three dimensions, the form of the distribution function upstream is:

\[
\begin{align*}
  f_{\text{dist}}(\mathbf{r}) &= \left( \frac{m}{2\pi k T_u} \right)^{\frac{3}{2}} \exp\left( -\frac{m((\dot{x} - V_u)^2 + \dot{y}^2 + \dot{z}^2)}{2kT_u} \right) \\
\end{align*}
\]  

The evolution of the distribution through the shock is determined by the Liouville equation:

\[
\begin{align*}
  \frac{\partial f}{\partial t} + \dot{x} \frac{\partial f}{\partial x} + \dot{y} \frac{\partial f}{\partial y} + \dot{z} \frac{\partial f}{\partial z} + p_1 \frac{\partial f}{\partial p_1} + p_2 \frac{\partial f}{\partial p_2} + p_3 \frac{\partial f}{\partial p_3} &= 0 \\
\end{align*}
\]  

where we have taken advantage of Hamilton's equations to obtain an expression in terms of the canonical momenta.

Note that the Liouville equation given in equation (3.18) is set in a 6-dimensional phase space, much like the Collisionless Boltzmann equation introduced in Chapter 1. The difference here is that we are concerned with a probability distribution - specifically, that of a single "test" particle which is affected by the motion of the other particles in the fluid only indirectly through the static and vector potentials - as opposed to the number density of a collection of particles. Thus, equation (3.18) is equivalent to equation (1.59) for \( N = 1 \).

For the remainder of the chapter, we consider only a steady state solution, and ignore the time derivative. The coefficients of this equation (which are the time
derivatives of the phase variables) give the tangent vector to the trajectory in phase space [EW03 and references therein]. The left hand side is the rate of change of $f$ along trajectories, and Liouville's equation tells us that $f$ is constant along trajectories. The coefficients are, by equations (3.3) and (3.4):

\[
\dot{x} = \frac{\partial H}{\partial p_1} = \frac{p_1}{m} 
\]

\[
\dot{y} = \frac{\partial H}{\partial p_2} = \frac{p_2 + B_x z - \alpha(x)}{m} 
\]

\[
\dot{z} = \frac{\partial H}{\partial p_3} = \frac{p_3}{m} 
\]

\[
\dot{p}_1 = -\frac{\partial H}{\partial x} = \frac{B_x(x)(p_2 + B_x z - \alpha(x))}{m} - \phi'(x) 
\]

\[
\dot{p}_2 = -\frac{\partial H}{\partial y} = V_u B_{uz} 
\]

\[
\dot{p}_3 = -\frac{\partial H}{\partial z} = \frac{-B_z(p_2 + B_z z - \alpha(x))}{m} 
\]

It can be shown that the form of $f_{dist}$ given in equation (3.17) is a solution to Liouville's equation upstream of the shock; we will revisit this later in the chapter.
3.2 Finding the Invariants of the Flow

The general solution to the steady state version of equation (3.18) is an arbitrary function of six invariants, functions of the position and momenta coordinates which are constant along trajectories [Sneddon, 1957]. We wish to write the distribution function in terms of these invariants. One invariant is the Hamiltonian, $H$, however, the distribution does not depend on $y$ and, as previously stated, the Hamiltonian cannot be the correct solution because the flow is not ergodic, so we seek another solution.

Since the Hamiltonian is linear in $y$, none of the partial derivatives of $H$ depend on $y$, and any solution (independent of $y$) to a reduced version of Liouville’s equation which ignores the $\frac{\partial f}{\partial y}$ term will also be a solution to the full Liouville equation [EW03 and references therein]. The other invariants are solutions to this reduced form:

$$\dot{x} \frac{\partial f}{\partial x} + \dot{z} \frac{\partial f}{\partial z} + \dot{p}_1 \frac{\partial f}{\partial p_1} + \dot{p}_2 \frac{\partial f}{\partial p_2} + \dot{p}_3 \frac{\partial f}{\partial p_3} = 0 \quad (3.25)$$

In order to find the invariants we follow Sneddon [1957]. The invariants are the constants of integration for the solution to the following set of differential equations:

$$\frac{dp_2}{V_u B_{ux}} = \frac{\hat{m} dx}{p_1} = \frac{\hat{m} dp_1}{B_z (p_2 + B_x z - \alpha(x)) - \hat{m} \phi'(x)}$$

$$\frac{\hat{m} dz}{p_3} = \frac{\hat{m} dp_3}{-B_x (p_2 + B_x z - \alpha(x))} \quad (3.26)$$

Using $p_2$ as the independent variable, we rewrite equations (3.26) as:

$$\frac{dx}{dp_2} = \frac{p_1}{\hat{m} V_u B_{ux}} \quad (3.27)$$
\[
\frac{dz}{dp_2} = \frac{p_3}{\hat{m}V_u B_{uz}}
\] (3.28)

\[
\frac{dp_1}{dp_2} = \frac{B_z(x)(p_2 + B_z z - \alpha(x)) - \hat{m}\phi'(x)}{\hat{m}V_u B_{uz}}
\] (3.29)

\[
\frac{dp_3}{dp_2} = \frac{-B_z (p_2 + B_z z - \alpha(x))}{\hat{m}V_u B_{uz}}
\] (3.30)

Clearly, we cannot write an explicit closed form for the solutions to these equations. However, if we can solve these equations far upstream of the shock (so that \(B_z(x), \alpha(x), \) and \(\phi'(x)\) are constant), we can define invariants in terms of the upstream solutions. For example, if \(K_u\) is a solution to the upstream Liouville equation, we define a function:

\[
K(x, y, z, p_1, p_2, p_3) = K_u(\hat{x}, \hat{y}, \hat{z}, \hat{p}_1, \hat{p}_2, \hat{p}_3)
\] (3.31)

such that a particle starting at \((\hat{x}, \hat{y}, \hat{z}, \hat{p}_1, \hat{p}_2, \hat{p}_3)\) in phase space will reach the point \((x, y, z, p_1, p_2, p_3)\) at some time along its trajectory. By definition, then, the function \(K\) is constant along trajectories, since at any point in phase space along the trajectory the function will have the value \(K_u(\hat{x}, \hat{y}, \hat{z}, \hat{p}_1, \hat{p}_2, \hat{p}_3)\).

In effect, the constants of integration found far upstream determine the initial conditions (or, equivalently, are determined by the initial conditions), and the invariant functions are defined such that they have the value of the corresponding upstream constant of integration along the same trajectory. In the same way, if we can express the upstream distribution function in terms of these upstream invariants (initial conditions), we can express the distribution function through and downstream of the shock in terms of our defined invariants. We can then investigate properties of the distribution using this expression.

Far upstream, equations (3.27) and (3.28) remain unchanged. For the latter two equations, we have \(\alpha(x) = B_{uz} x\) and \(\phi'(x) = 0\), so equations (3.29) and (3.30) simplify to:
3.2.1 Decoupling the Differential Equations

We seek a solution to equations (3.27), (3.28), (3.32), and (3.33), which will determine the upstream form of the invariants. We first introduce a surrogate for $p_2$, with $u = p_2 - p_2(0)$, in order to make the system autonomous. Now, with $p = [x, z, u, p_1, p_3]^T$ we have:

$$
\frac{dp_3}{dp_2} = \frac{-B_z(p_2 + B_2 z - B_u z)}{\hat{m} V_u B_u z}
$$

(3.33)

The eigenvalues of $K$ are $\lambda = 0, 0, 0, i|B_u|, -i|B_u|$, where $|B_u|^2 = B_u^2 + B_z^2$. We wish to diagonalize this matrix, decoupling the differential equations. However:
Since the geometric multiplicity (dimension of the kernel, or null space, of \( K - \lambda I \)) of the eigenvalue 0 is 2, while the algebraic multiplicity is 3, \( K \) is a defective matrix (not diagonalizable). Instead, we seek the Jordan normal form, \( K = MDM^{-1} \). The matrix \( D \) is "almost" diagonal; the only non-zero elements lie on the main diagonal or the superdiagonal of the matrix.

The transformation matrix, \( M \), is formed of the eigenvectors. To find the third (generalized) eigenvector associated with eigenvalue 0, we require a vector \( v_2 \) such that \((K - 0I)v_2 = v_1\), where \( v_1 \) is an ordinary eigenvector. Since the third row of \( K \) is everywhere 0, the third element of \( v_1 \) must likewise be 0, regardless of what \( v_2 \) is, so we choose an eigenvector in the span given in equation (3.37) with this constraint:

\[
\begin{bmatrix}
B_x \\
B_{uz} \\
0 \\
0 \\
0
\end{bmatrix}
\]

(3.38)

Then, one solution for \( v_2 \) is:

\[
\begin{bmatrix}
0 \\
0 \\
0 \\
0 \\
B_x \\
B_{uz}
\end{bmatrix}
\]

(3.39)

These vectors correspond to the first Jordan block. The second Jordan block also corresponds to the eigenvalue 0, so we require another eigenvector independent of \( v_1 \); for example:
For the other two eigenvalues we have the associated eigenvectors:

\[
\mathbf{v}_4 = \begin{bmatrix}
B_{uz} \\
-B_x \\
0 \\
iB_{uz}|B_u| \\
-iB_x|B_u|
\end{bmatrix}
\] (3.41)

\[
\mathbf{v}_5 = \begin{bmatrix}
B_{uz} \\
-B_x \\
0 \\
-iB_{uz}|B_u| \\
iB_x|B_u|
\end{bmatrix}
\] (3.42)

Now, \( K = MDM^{-1} \), where:

\[
D = \begin{bmatrix}
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & i|B_u| & 0 \\
0 & 0 & 0 & 0 & -i|B_u|
\end{bmatrix}
\] (3.43)

This matrix is formed of Jordan blocks along the diagonal (with 0 elsewhere). Here, we have three 1 \( \times \) 1 Jordan blocks, each of which contains the associated eigenvalue as its lone element, along with an additional 2 \( \times \) 2 block (top left) for the eigenvalue 0, which has a geometric multiplicity of 2 (two Jordan blocks) and an algebraic multiplicity of 3 (equalling the sum of the dimensions of the
two Jordan blocks). This Jordan block contains elements equal to the eigenvalue along the main diagonal, 1 along the superdiagonal, and 0 elsewhere.

The matrix $M$ is formed by putting the eigenvectors (and generalized eigenvector) together in order:

$$
M = \begin{bmatrix}
B_x & 0 & 1 & B_{uz} & B_{uz} \\
B_{uz} & 0 & 0 & -B_x & -B_x \\
0 & 0 & B_{uz} & 0 & 0 \\
0 & B_x & 0 & iB_{uz}|B_u| & -iB_{uz}|B_u| \\
0 & B_{uz} & 0 & -iB_x|B_u| & iB_x|B_u|
\end{bmatrix}
$$

(3.44)

and we find that the inverse of this matrix is:

$$
M^{-1} = \frac{1}{2|B_u|^2} \begin{bmatrix}
2B_x & 2B_{uz} & \frac{2B_x}{B_{uz}} & 0 & 0 \\
0 & 0 & 0 & 2B_x & 2B_{uz} \\
0 & 0 & \frac{2|B_u|^2}{B_{uz}} & 0 & 0 \\
B_{uz} & -B_x & -1 & \frac{-iB_{uz}}{|B_u|} & \frac{iB_x}{|B_u|} \\
B_{uz} & -B_x & -1 & \frac{iB_{uz}}{|B_u|} & \frac{-iB_x}{|B_u|}
\end{bmatrix}
$$

(3.45)

We can now decouple the differential equations by substituting $\dot{p} = M^{-1}p$. Equation (3.34) becomes:

$$
\dot{m}V_uB_{uz}\frac{d\dot{p}}{dp_2} = D\dot{p} + s
$$

(3.46)

where:

$$
D\dot{p} = \begin{bmatrix}
\dot{p}_2 \\
0 \\
0 \\
i|B_u|\dot{p}_4 \\
-i|B_u|\dot{p}_5
\end{bmatrix}
$$

(3.47)
\[ s = M^{-1}r \]
\[ = \begin{bmatrix}
-\hat{m}V_u B_x \\
\frac{-\hat{m}V_u B_u}{|B_u|^2} \\
0 \\
\frac{-\hat{m}V_u B_u - ip_2(0)}{2|B_u|^2} \\
\frac{-\hat{m}V_u B_u + ip_2(0)}{2|B_u|^2}
\end{bmatrix} \] (3.48)

(This transformation is not canonical, since $|M| \neq 1$. Since any scalar multiple of one of the eigenvectors comprising $M$ is also an eigenvector, we could choose eigenvectors such that $|M| = 1$ and the transformation is canonical, but this is unnecessary for the calculation of the invariants.)

### 3.2.2 Solving for the Invariants Upstream

We now consider the resulting equations (3.46), solving for the variables $\hat{p}_1$. Starting with $\hat{p}_2$:

\[ \hat{m}V_u B_u \frac{d\hat{p}_2}{dp_2} = 0 \]
\[ \Rightarrow \hat{p}_2 = \text{constant} \] (3.49)

In fact, from $\hat{p} = M^{-1}p$ we have:

\[ \hat{p}_2 = \frac{B_x p_1 + B_{u_2} p_3}{|B_u|^2} \] (3.50)

Then, substituting into the equation for $\hat{p}_1$:

\[ \hat{m}V_u B_u \frac{d\hat{p}_1}{dp_2} = \hat{p}_2 - \frac{\hat{m}V_u B_x}{|B_u|^2} \]
\[ = \frac{B_x (p_1 - \hat{m}V_u) + B_{u_2} p_3}{|B_u|^2} \] (3.51)

The right hand side is constant, and we choose this form for the invariant $I_u$:

\[ |B_u|^2 I_u = B_x (p_1 - \hat{m}V_u) + B_{u_2} p_3. \] (Note that here, and throughout this section,
we use $I_u$ to represent the form of the invariant $I$ in terms of the upstream phase variables, and similarly with the other invariants. $I$ is constant along trajectories, but does not retain this form with respect to the phase variables through the shock.)

$$\dot{p}_1 = \left( \frac{I_u}{\hat{m} V_u B_{uz}} \right) p_2 + C_1 \tag{3.52}$$

where $C_1$ is a second constant of integration (invariant). Next:

$$\hat{m} V_u B_{uz} \frac{d\hat{p}_3}{dp_2} = \hat{m} V_u \tag{3.53}$$

which gives $\dot{p}_3 = \frac{p_2}{B_{uz}} + C_2$. From $p = M\dot{p}$ we have $u = B_{uz}\dot{p}_3$, so $C_2 = -\frac{p_2(0)}{B_{uz}}$.

The final two equations are:

$$\hat{m} V_u B_{uz} \frac{d\hat{p}_4}{dp_2} = i|B_u|\dot{p}_4 - \frac{\hat{m} V_u B_{uz} + i p_2(0)}{2|B_u|^2} \tag{3.54}$$

and:

$$\hat{m} V_u B_{uz} \frac{d\hat{p}_5}{dp_2} = i|B_u|\dot{p}_5 - \frac{\hat{m} V_u B_{uz} - i p_2(0)}{2|B_u|^2} \tag{3.55}$$

This pair of equations results in:

$$\dot{p}_4 = C_3 \exp \left( \frac{i|B_u|}{\hat{m} V_u B_{uz}} p_2 \right) + \frac{p_2(0) - i\hat{m} V_u B_{uz}}{2|B_u|^3} \tag{3.56}$$

$$\dot{p}_5 = C_4 \exp \left( -\frac{i|B_u|}{\hat{m} V_u B_{uz}} p_2 \right) + \frac{p_2(0) + i\hat{m} V_u B_{uz}}{2|B_u|^3} \tag{3.57}$$

Now, we can again use $p = M\dot{p}$ to obtain equations for the canonical position and momentum variables.
We require that \( x \) and \( z \) are real. Note that:

\[
C_3 \exp(i\theta) + C_4 \exp(-i\theta) = (C_3 + C_4) \cos(\theta) + (C_3 - C_4)i \sin(\theta)
\]

(3.59)

and:

\[
C_5 \cos(\theta - \Psi_u) = C_5 (\cos(\theta) \cos(\Psi_u) + \sin(\theta) \sin(\Psi_u))
\]

(3.60)

By substituting \( C_3 = \frac{C_5 \cos(\Psi_u) - i \sin(\Psi_u)}{2} \) and \( C_4 = \frac{C_5 \cos(\Psi_u) + i \sin(\Psi_u)}{2} \), we obtain the latter form for real \( C_5 \) and \( \Psi_u \). Gathering terms yields:

\[
x = \left( \frac{B_x I_u + \hat{m} V_u}{\hat{m} V_u B_{uz}} \right) p_2 + B_x C_u + B_{uz} C_5 \cos \left( \frac{|B_u|}{\hat{m} V_u B_{uz}} p_2 - \Psi_u \right)
\]

(3.61)

where \( C_u = C_1 - \frac{B_x p_2(0)}{B_{uz} |B_u|^2} \). Likewise, for \( z \):

\[
z = B_{uz} \hat{p}_1 - B_x (\hat{p}_4 + \hat{p}_5)
\]

\[
= \left( \frac{I_u}{\hat{m} V_u} \right) p_2 + B_{uz} C_u - B_x C_5 \cos \left( \frac{|B_u|}{\hat{m} V_u B_{uz}} p_2 - \Psi_u \right)
\]

(3.62)

From (3.27) and (3.28) we can find expressions for the momenta.

\[
p_1 = B_x I_u + \hat{m} V_u - B_{uz} |B_u| C_5 \sin \left( \frac{|B_u|}{\hat{m} V_u B_{uz}} p_2 - \Psi_u \right)
\]

(3.63)

\[
p_3 = B_{uz} I_u + B_x |B_u| C_5 \sin \left( \frac{|B_u|}{\hat{m} V_u B_{uz}} p_2 - \Psi_u \right)
\]

(3.64)
We now seek expressions for \( C_u, C_5, \) and \( \Psi_u \) in terms the upstream phase variables. Multiplying the expressions for \( x \) and \( z \), equations (3.61) and (3.62), by \( B_x \) and \( B_{uz} \) respectively and summing, we have:

\[
B_x x + B_{uz} z = \left( \frac{|B_u|^2 I_u + \tilde{m} V_u B_z}{\tilde{m} V_u B_{uz}} \right) p_2 + |B_u|^2 C_u \quad (3.65)
\]

\[
|B_u|^2 C_u = \frac{\tilde{m} V_u B_{uz} (B_x x + B_{uz} z) - p_2(B_x p_1 + B_{uz} p_3)}{\tilde{m} V_u B_{uz}} \quad (3.66)
\]

We can rewrite the expressions for \( x \) and \( p_1 \), equations (3.61) and (3.63), as:

\[
B_{uz} C_5 \cos \left( \frac{|B_u|}{\tilde{m} V_u B_{uz}} p_2 - \Psi_u \right) = x - \left( \frac{B_x I_u + \tilde{m} V_u}{\tilde{m} V_u B_{uz}} \right) p_2 - B_x C_u
\]

\[
= \frac{B_{uz} (B_{uz} x - B_x z - p_2)}{|B_u|^2} \quad (3.67)
\]

\[
-B_{uz} C_5 \sin \left( \frac{|B_u|}{\tilde{m} V_u B_{uz}} p_2 - \Psi_u \right) = \frac{p_1 - B_x I_u - \tilde{m} V_u}{|B_u|} \]

\[
= \frac{B_{uz} (B_{uz} (p_1 - \tilde{m} V_u) - B_x p_3)}{|B_u|^3} \quad (3.68)
\]

Squaring these equations, summing, and simplifying gives:

\[
|B_u|^6 C_5^2 = (B_{uz} (p_1 - \tilde{m} V_u) - B_x p_3)^2 + |B_u|^2 (p_2 + B_x z - B_{uz} x)^2
\]

\[
= |B_u|^4 \rho_u^2 \quad (3.69)
\]

where \( \rho_u \) is the upstream gyroradius of the ion (see Appendix C for a derivation of upstream gyroradius in terms of the upstream phase variables). Thus, \( |B_u| C_5 = \rho_u \).

If we divide equation (3.68) by (3.67) instead of squaring and summing, we obtain an expression for \( \Psi_u \).
In summary, the upstream phase variables are, in terms of the four invariant forms chosen \( \langle I, \rho, C, \text{ and } \Psi \rangle \):

\[
\begin{align*}
\tan \left( \frac{|B_u|p_2}{\hat{m}V_u B_{uz}} - \Psi_u \right) &= \frac{B_{uz}(p_1 - \hat{m}V_u) - B_z p_3}{|B_u|(p_2 + B_z z - B_{uz} x)} \tag{3.70} \\
\Psi_u &= \frac{|B_u|p_2}{\hat{m}V_u B_{uz}} - \arctan \left( \frac{B_{uz}(p_1 - \hat{m}V_u) - B_z p_3}{|B_u|(p_2 + B_z z - B_{uz} x)} \right) \tag{3.71}
\end{align*}
\]

If we consider what the invariants "mean" upstream of the shock in this context of the invariants determining the upstream phase variables (rather than vice versa), \( I \) relates to the guiding centre trajectory of the ion, \( \rho \) is the upstream gyroradius, \( \Psi \) is an angle along that gyration, and \( C \) gives the position in the \( xz \)-plane. Another constant of integration, denoted \( C_2 \) above, determines the value of \( p_2 \) at \( t = 0 \). The Hamiltonian completes the set of six invariants, and its value determines \( y \).

(Appendix D offers an alternative method for solving for the invariants by solving a fourth-order partial differential equation as opposed to the decoupling method given here. Appendix E shows how the decoupling method might be used through the shock.)
Note that:

\[ |B_u|^2(p_u^2 + I_u^2) = (p_1 - \hat{m}V_u)^2 + (p_2 + B_uz - B_u x)^2 + p_3^2 \]
\[ = \hat{m}^2((\hat{x} - V_u)^2 + \hat{y}^2 + \hat{z}^2) \]
\[ = |B_u|^2S^2_u \quad (3.76) \]

where \( S_u \) is the generalization to three dimensions of the upstream form of the invariant used in EW03 (for a quasi-perpendicular shock, \( S_u \) and \( \rho_u \) are no longer equivalent). As stated previously, any function of the invariants is also an invariant of the flow and a solution to Liouville's equation. In particular:

\[ f = \left( \frac{q^2}{2\pi m kT_u} \right)^{\frac{3}{2}} \exp \left( -\frac{q^2|B_u|^2S^2}{2kT_u} \right) \quad (3.77) \]

is a solution. Comparing with equation (3.17), we see that this solution matches the upstream boundary condition of a Maxwellian distribution. Surfaces of constant \( f \) are spheres with radius \( |B_u|S \) in phase space, and \( S, I, \) and \( \Psi \) comprise a cylindrical coordinate system which we will make use of in the next section.

If we begin with an ensemble of ions and follow these ions along their trajectories, we have two related issues. We are interested in snapshots of the velocity distribution within or downstream of the shock at particular values of \( x \) (which is the distance normal to the shock); however, a distribution of ions starting from the same location will become spread out not only in velocity space, but in physical space as well. Additionally, while \( p_1 \) and \( p_3 \) are proportional to the corresponding velocities, \( \hat{x} \) and \( \hat{z} \), the relationship between \( p_2 \) and \( \hat{y} \) shows a dependence on both \( x \) and \( z \).

To account for this, we note that for a system which varies only in \( x \) - that is, the fields and ion distributions are independent of the other position coordinates - we can consider equivalence classes of ion trajectories by ignoring \( y \) and \( z \) position. Ions reaching a given physical position with different velocities will have started out at different initial positions, but we are only concerned with the spread of velocities for a given "snapshot" of the distribution. Therefore, for the remainder of the chapter, we will make the substitution.
\[ p_4 = \dot{m} \dot{y} = p_2 + B_2 z - \alpha(x), \] and will consider phase shells in \( p_1 p_4 p_3 \)-space (effectively, velocity space) rather than \( p_1 p_2 p_3 \)-space.

### 3.3 Evolution of Distribution Properties Through the Shock

We can now make use of the invariants found in the previous section to find various moments of the distribution (average momenta/velocities and temperature/pressure components), as well as calculate the phase volume contained within surfaces of constant probability. The phase volume is related to the temperature, which is a measure of the variance of the distribution in velocity space - thus, by finding an expression for the evolution of the phase volume, we gain an understanding of the heating which takes place through the low Mach number quasi-perpendicular shock, despite the absence of collisions, reflected ions, turbulence, or other dissipation.

We can find the phase volume of a given distribution of ions by integrating over the phase variables (momenta). This is of little analytical use through the shock, as we do not have analytical solutions for the trajectories. Instead, we wish to write the volume integral in terms of the invariants which are functions of the momenta only (far upstream of the shock): \( S, I, \) and \( \Psi \). We do this by using the Jacobian, \( J \), which is the matrix of partial derivatives:

\[
J = \begin{bmatrix}
\frac{\partial p_1}{\partial \Psi} & \frac{\partial p_1}{\partial I} & \frac{\partial p_1}{\partial S} \\
\frac{\partial p_2}{\partial \Psi} & \frac{\partial p_2}{\partial I} & \frac{\partial p_2}{\partial S} \\
\frac{\partial p_3}{\partial \Psi} & \frac{\partial p_3}{\partial I} & \frac{\partial p_3}{\partial S}
\end{bmatrix}
\] (3.78)

Then:

\[
dp_1 dp_4 dp_3 = |J| d\Psi dI dS
\] (3.79)
3.3.1 Calculation of the Jacobian

To solve for det(J), we first rewrite equations (3.26), this time using \( x \) as the independent variable [c.f., EW03].

\[
\frac{dp_1}{dx} = \frac{B_z(x)p_4 - \dot{m}\phi'(x)}{p_1}
\]

(3.80)

\[
\frac{dp_4}{dx} = \frac{\dot{m}V_u B_{ux}}{p_1}
\]

(3.81)

\[
\frac{dp_3}{dx} = -\frac{B_z p_4}{p_1}
\]

(3.82)

Differentiating these with respect to \( \Psi \) gives:

\[
\frac{d}{dx} \frac{\partial p_1}{\partial \Psi} = \frac{B_z(x)}{p_1} \frac{\partial p_4}{\partial \Psi} - \frac{B_z(x)p_4 - \dot{m}\phi'(x)}{p_1^2} \frac{\partial p_1}{\partial \Psi}
\]

(3.83)

\[
\frac{d}{dx} \frac{\partial p_4}{\partial \Psi} = -\frac{\dot{m}V_u B_{ux}}{p_1^2} \frac{\partial p_1}{\partial \Psi}
\]

(3.84)

\[
\frac{d}{dx} \frac{\partial p_3}{\partial \Psi} = \frac{-B_z \partial p_4}{p_1 \partial \Psi} + \frac{B_z p_4 \partial p_1}{p_1^2 \partial \Psi}
\]

(3.85)

with similar equations obtained by differentiating with respect to the other invariants.

Now, let \( \Gamma = |J| \) and consider \( \frac{d\Gamma}{dx} \). We can write this as the sum of three determinants, where each determinant is of a matrix \( J_i \) which is identical to \( J \) except that the elements of row \( i \) are differentiated with respect to \( x \). The second and third determinants, \(|J_2|\) and \(|J_3|\), are equal to 0, since by the above equations the rows are not linearly independent. We are left with:
Again we see that in the first determinant, the first two rows are not linearly independent, and this determinant is 0. Taking out the factor $\frac{\partial dp_1}{dp_1 dx}$ in the second determinant, we are left with:

\[
\frac{d\Gamma}{dx} = \frac{\partial}{\partial p_1} \frac{dp_1}{dx} \Gamma
\]

\[
= -\frac{B_s(x)p_4 - \dot{m}\delta'(x)}{p_1^2} \Gamma
\]

(3.87)

Then:

\[
\frac{d\Gamma}{dx} = -\frac{B_s(x)p_4 - \dot{m}\delta'(x)}{p_1^2}
\]

\[
\frac{1}{\Gamma} \frac{d\Gamma}{dx} = -\frac{1}{p_1} \frac{dp_1}{dx}
\]

(3.88)

Therefore:

\[
\frac{d\ln \Gamma}{dx} = -\frac{d\ln p_1}{dx}
\]

\[
\Rightarrow \Gamma = \frac{K(S, I, \Psi)}{p_1}
\]

(3.89)

where $K$ is independent of $x$. We can obtain $K$ by evaluating $|J^{-1}| = \frac{1}{\Gamma}$ far upstream. Noting that $\det(J^{-1})dp_1dp_4dp_3 = d\Psi dIdS$, we have:
\[ |J^{-1}| = \begin{vmatrix} \frac{\partial \psi}{\partial p_1} & \frac{\partial \psi}{\partial p_4} & \frac{\partial \psi}{\partial p_3} \\ \frac{\partial I}{\partial p_1} & \frac{\partial I}{\partial p_4} & \frac{\partial I}{\partial p_3} \\ \frac{\partial S}{\partial p_1} & \frac{\partial S}{\partial p_4} & \frac{\partial S}{\partial p_3} \end{vmatrix} = \frac{B_z}{|B_u|^2} \begin{vmatrix} \frac{\partial \psi}{\partial p_1} & \frac{\partial \psi}{\partial p_4} & \frac{\partial \psi}{\partial p_3} \\ \frac{\partial S}{\partial p_1} & \frac{\partial S}{\partial p_4} & \frac{\partial S}{\partial p_3} \end{vmatrix} - \frac{B_{uz}}{|B_u|^2} \begin{vmatrix} \frac{\partial S}{\partial p_1} & \frac{\partial S}{\partial p_4} \\ \frac{\partial S}{\partial p_1} & \frac{\partial S}{\partial p_4} \end{vmatrix} \] (3.90)

The partial derivatives are:

\[ \frac{\partial S}{\partial p_1} = \frac{(p_1 - \bar{m}V_u)}{|B_u|^2S} \] (3.91)

\[ \frac{\partial S}{\partial p_4} = \frac{p_4}{|B_u|^2S} \] (3.92)

\[ \frac{\partial S}{\partial p_3} = \frac{p_3}{|B_u|^2S} \] (3.93)

\[ \frac{\partial \Psi}{\partial p_1} = \frac{-B_{uz}|B_u|p_4}{|B_u|^4(S^2 - I^2)} \] (3.94)

\[ \frac{\partial \Psi}{\partial p_4} = \frac{|B_u|}{\bar{m}V_u B_{uz}} + \frac{|B_u|(B_{uz}(p_1 - \bar{m}V_u) - B_xp_3)}{|B_u|^4(S^2 - I^2)} \] (3.95)

\[ \frac{\partial \Psi}{\partial p_3} = \frac{B_x|B_u|p_4}{|B_u|^4(S^2 - I^2)} \] (3.96)

where [c.f., equations (3.69) and (3.76)]:

\[ |B_u|^4(S^2 - I^2) = (B_{uz}(p_1 - \bar{m}V_u) - B_xp_3)^2 + |B_u|^2p_4^2 \] (3.97)
Rearranging the determinants, we have:

\[
J^{-1} = \frac{\partial S}{\partial p_4} \left( \frac{B_x}{|B_u|^2} \frac{\partial \Psi}{\partial p_4} - \frac{B_{uxz}}{|B_u|^2} \frac{\partial \Psi}{\partial p_1} \right) \\
+ \frac{\partial \Psi}{\partial p_4} \left( \frac{B_{uz}}{|B_u|^2} \frac{\partial S}{\partial p_4} - \frac{B_x}{|B_u|^2} \frac{\partial S}{\partial p_3} \right) \\
= \frac{|B_u|^2 p_4^2}{|B_u|^3 S(S^2 - I^2)} + \frac{(B_{uz}(p_1 - \hat{m}V_u) - B_{z}p_3)^2}{|B_u|^3 S(S^2 - I^2)} \\
+ \frac{B_{uz}(p_1 - \hat{m}V_u) - B_{z}p_3}{\hat{m}V_u B_{uz} |B_u|^3 S} \\
= \frac{1}{|B_u|^3 S} + \frac{B_{uz}(p_1 - \hat{m}V_u) - B_{z}p_3}{\hat{m}V_u B_{uz} |B_u|^3 S} \\
= \frac{B_{uz}p_1 - B_{z}p_3}{\hat{m}V_u B_{uz} |B_u|^3 S} \\
= \frac{\hat{m}V_u B_{uz} |B_u|^3 S}{B_{uz}p_1 - B_{z}p_3}
\] (3.98)

And so:

\[
\Gamma = \frac{\hat{m}V_u B_{uz} |B_u|^3 S}{B_{uz}p_1 - B_{z}p_3} \\
\Rightarrow K = \frac{\hat{m}V_u |B_u|^3 S}{B_{uz}p_1 - B_{z}p_3}
\] (3.99)

This form of \( K \) is valid upstream. However, \( K \) is a constant function of the invariants, while through the shock \( p_1 \) and \( p_3 \) are not constant, so this form is not valid through the shock. Fortunately, as we will see in the next section, the exact form of \( K \) is not necessary in the calculation of the phase volume.

### 3.3.2 Phase Volume

For fixed \( x \), let \( \Lambda_x(S_{\text{max}}) \) be the volume in phase space enclosed by the surface \( S = S_{\text{max}} \). Then, using equations (3.79) and (3.89):

\[
\Lambda_x(S_{\text{max}}) = \int \int \int _{S \leq S_{\text{max}}} dP_1 dP_4 dP_3 \\
= \int _{S_{\text{max}}} ^{S} \int _{-S} ^{S} \int _{P_1} ^{2\pi} \frac{K}{P_1} d\Psi dI dS
\] (3.100)
Here, $K$ is a function of the three invariants only, while $p_1$ depends on the invariants and on the position, $x$. Let $p_1^*$ represent the average value of $p_1$ over the volume, without regard to the probability distribution. We have:

\[
p_1^* = \frac{\int_0^{S_{\text{max}}} \int_S^{2\pi} p_1 K d\Psi dS}{\int_0^{S_{\text{max}}} \int_S^{2\pi} p_1 d\Psi dS} = \frac{\int_0^{S_{\text{max}}} \int_S^{2\pi} K d\Psi dS}{A_x(S_{\text{max}})} \tag{3.101}
\]

The numerator on the right-hand side is constant through the shock. We can therefore evaluate it far upstream, taking advantage of the knowledge that the upstream phase shell is a sphere of radius $|B_u|S_{\text{max}}$ and, by symmetry, $p_1^* = \bar{n}V_u$, the upstream modal trajectory:

\[
\int_0^{S_{\text{max}}} \int_S^{2\pi} K d\Psi dS = p_1^* A_u(S_{\text{max}}) = \frac{4\pi \bar{n}V_u(|B_u|S_{\text{max}})^3}{3} \tag{3.102}
\]

Substituting this into equation (3.101) and rearranging, we can write the volume through the shock as:

\[
A_x(S_{\text{max}}) = \frac{4\pi \bar{n}V_u(|B_u|S_{\text{max}})^3}{3p_1^*} \tag{3.103}
\]

We can see this result more directly for small $S$ by noting that the relative variation from the bulk velocity is small. Thus, we assume $p_1 >> p_3$, and, from equation (3.99):

\[
K \approx \bar{n}V_u |B_u|^3 S \tag{3.104}
\]

Then, using the Integral Mean Value Theorem to extract an intermediate value of $p_1$, we find:
In the limit, we have:

\[
\lim_{S_{\text{max}} \to 0} \frac{3 \Lambda_x(S_{\text{max}})}{4\pi \left(||B_u||S_{\text{max}}\right)^3} = \frac{\dot{m}V_u}{\bar{p}_1}
\] (3.106)

where \(\bar{p}_1\) is the value of \(p_1\) corresponding to the modal trajectory (\(S = 0\), with \(p_1 = \dot{m}V_u\) upstream of the shock). This generalizes the result of EW03, equation (3.1), to three dimensions.

### 3.3.3 Mean and Variance of the Downstream Distribution

The phase volume is an integral over the invariants which does not take into account the probability distribution of the trajectories, and it is also limited to a finite range of initial parameters. Thus, \(p_1^*\) as defined above is not exactly equal to the mean of the distribution (though, as we will see later, it does serve as a good approximation).

As discussed briefly in section 1.1.5, we can calculate various bulk properties of a distribution (the number density, mean velocity, and kinetic temperature/pressure) using moments of the distribution. For a given function, \(g\):

\[
\langle g \rangle = \frac{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(f(p))dp_1dp_4dp_3}{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(p)dp_1dp_4dp_3}
\] (3.107)

The notation \(\langle g \rangle\) represents the expected value (the mean) of \(g\) over the distribution. Note that for the system under investigation, we don't know the
form of $f(p)$ through the shock. However, since we can express the probability distribution in terms of the invariant $S$, we can use the Jacobian and a change of coordinates to obtain a form usable through the shock. For example, the mean value of $p_1$ can be found by the following equation:

$$\bar{p}_1 \equiv \langle p_1 \rangle = \frac{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} p_1 f(p) dp_1 dp_2 dp_3}{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(p) dp_1 dp_2 dp_3} = \frac{\int_{0}^{\infty} f(p) \int_{-S}^{S} \int_{0}^{2\pi} K d\Psi dI dS}{\int_{0}^{\infty} f(p) \int_{-S}^{S} \int_{0}^{2\pi} \frac{K}{p_1} d\Psi dI dS}$$

(3.108)

where $f$, the distribution given by equation (3.77), is independent of $I$ and $\Psi$ and can be taken out of the innermost integrals. Note that the denominator of equation (3.108) is not constant, since the probability distribution is normalized with respect to the upstream velocity. Far upstream, however, the denominator is 1; it is the integral of the normalized Maxwellian probability distribution over the entire phase space. Also, the mean value of $p_1$ (upstream) is $\bar{m}V_u$. Thus, upstream we have that the numerator is also $\bar{m}V_u$ and since $K$ is a function of the invariants only, the numerator is constant:

$$\bar{p}_1 = \frac{\bar{m}V_u}{\int_{0}^{\infty} f(p) \int_{-S}^{S} \int_{0}^{2\pi} \frac{K}{p_1} d\Psi dI dS}$$

(3.109)

Naturally, this expression is similar to equation (3.101); the mean value, $\bar{p}_1$ takes into account the probability distribution, while the value $p_1$ is the average value of $p_1$ over the points of velocity space contained within the chosen phase shell.

In calculating the mean numerically, we might consider using a Gauss-Laguerre quadrature method to evaluate the denominator. However, while only a small portion of the distribution is reflected from the shock, the integral here is over the entire distribution, including these backstreaming ions; since the integrand contains a $\frac{1}{p_1}$ term, we will see asymptotic behaviour for sufficiently large $S$, possibly affecting the accuracy of the quadrature method. Because these values are unlikely, we can obtain a good estimate for the average momenta values by setting the upper limit of the integral to a sufficiently high (but finite) value of $S$. 

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S. The effect of this limitation on the calculated temperature will be discussed in the context of the numerical results in Section 3.4.3.

We find the temperature of the distribution in a similar manner. As noted in Section 1.1.5, for a distribution in thermodynamic equilibrium - that is, a Maxwellian distribution - we can attribute a single temperature value, since the distribution is isotropic. However, for an anisotropic distribution, we require a more general definition of the temperature.

We define the temperature tensor such that the components are proportional to the second moments in the corresponding pair of directions - that is, \( T_{xx} \) is proportional to the variance from the mean in \( v_x \), and similarly for other directions.

The total temperature is then the trace of the tensor, and is proportional to the sum of the second moments of the velocities about their mean values [EW06]:

\[
T = \frac{1}{3} (T_{xx} + T_{yy} + T_{zz}) = \frac{q^2}{3mk} \left[ \langle p_1^2 + p_2^2 + p_3^2 \rangle - \langle \bar{p}_1^2 + \bar{p}_2^2 + \bar{p}_3^2 \rangle \right]
\]

\[
\Rightarrow \frac{3kT}{2} = \frac{1}{2} m \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(v) \times ( (v_x - \bar{v}_x)^2 + (v_y - \bar{v}_y)^2 + (v_z - \bar{v}_z)^2 ) \, dv_x \, dv_y \, dv_z
\]

where \( v_x = \dot{x} \) is the x-component of the velocity (and similarly for the other components). With this last expression, we can see the relationship between the temperature and the kinetic energy of an individual particle, \( KE = \frac{1}{2} m v^2 \).

To investigate the temperature anisotropy, we define the temperature tensor which generalizes the above relationship between the temperature and the variance. The component of the temperature tensor in the \( x \) direction is:

\[
T_{xx} = \frac{q^2}{mk} \left[ \langle p_1^2 \rangle - \bar{p}_1^2 \right]
\]

and likewise for the other directions, with:
For the off-diagonal elements of the temperature tensor, we have:

\[ T_{xy} = T_{yx} = \frac{q^2}{mk} \left[ \langle p_1 p_4 \rangle - \bar{p}_1 \bar{p}_4 \right] \]  

(3.113)

and similarly for the other components.

We are also interested in the temperatures perpendicular and parallel to the magnetic field, in order to study the \( T_L > T_{||} \) anisotropy [e.g., Thomsen et al., 1985; Wilkinson, 1991; Gedalin, 1996b, 1997]. Let \( \hat{b} \) be the direction parallel to the magnetic field, and let \( \hat{k} = \hat{b} \times \hat{y} \) complete the new coordinate system as a direction in the \( xz \)-plane perpendicular to the magnetic field (we retain \( \hat{y} \), which is also perpendicular to the magnetic field, as the third vector). Let \( p_b \) and \( p_k \) be momenta in these directions:

\[ p_b = \frac{B_x}{|B|} p_1 + \frac{B_z}{|B|} p_3 \]  

(3.114)

\[ p_k = \frac{B_x}{|B|} p_3 - \frac{B_z}{|B|} p_1 \]  

(3.115)

The corresponding temperatures are then:

\[ T_{bb} = \frac{q^2}{mk} \left[ \langle p_b^2 \rangle - \langle p_b^2 \rangle \right] \]

\[ = \frac{q^2}{mk} \left[ \left( \frac{B_x}{|B|} p_1 + \frac{B_z}{|B|} p_3 \right)^2 - \left( \frac{B_x}{|B|} \bar{p}_1 + \frac{B_z}{|B|} \bar{p}_3 \right)^2 \right] \]

\[ = \frac{B_x^2}{|B|^2} T_{xx} + \frac{2 B_x B_z}{|B|^2} T_{xz} + \frac{B_z^2}{|B|^2} T_{zz} \]  

(3.116)

and similarly:

\[ T_{kk} = \frac{B_z^2}{|B|^2} T_{zz} - 2 \frac{B_x B_z}{|B|^2} T_{xz} + \frac{B_z^2}{|B|^2} T_{zz} \]  

(3.117)
3.4 Comparison with Numerical Results

We now use numerically calculated trajectories to investigate the shape of shells of \( S^2 = \) constant through the shock, the phase volume of these shells, and the temperature of the distribution. For the fields, a typical shock profile model is used [e.g. Lee et al., 1986; Gedalin, 1996b; EW03; EW07]. The magnetic field is given by:

\[
B_z(x) = \frac{B_{dz} + B_{uz}}{2} \tan \left( \frac{x}{\lambda} \right) + \frac{B_{dz} - B_{uz}}{2} \tanh \left( \frac{x}{\lambda} \right) \tag{3.118}
\]

where \( B_{uz} \) and \( B_{dz} \) are the upstream and downstream \( z \) components of the magnetic field and \( \lambda \) is a parameter determining the width of the shock. Then:

\[
\alpha(x) = \left[ \int_{x_0}^{x} B_z \, dx \right] \left[ \frac{B_{dz} + B_{uz}}{2} (x - x_0) + \frac{B_{dz} - B_{uz}}{2} \lambda \ln \left( \frac{\cosh (\frac{x}{\lambda})}{\cosh (\frac{x_0}{\lambda})} \right) \right] \tag{3.119}
\]

where \( x_0 \) is the initial value of \( x \), and the constant of integration is chosen so that \( \alpha(x_0) = 0 \). The \( x \)-component of the magnetic field is constant, and is given by \( B_x = B_{uz} \cot \theta_{bn} \). The electrostatic potential is:

\[
\phi(x) = \phi_{\text{max}} \frac{1 + \tanh \left( \frac{x}{\lambda} \right)}{2} \tag{3.120}
\]

and we have:

\[
\phi'(x) = \phi_{\text{max}} \frac{\text{sech}^2 \left( \frac{x}{\lambda} \right)}{2\lambda} \tag{3.121}
\]

We use the following parameters: \( \hat{m} = 1.044 \times 10^{-10} \text{kg} \) (the mass and charge are those of a proton), \( V_u = 4 \times 10^5 \text{m} \), \( B_{uz} = 20 \text{nT} \), and \( B_{dz} = 40 \text{nT} \). We choose \( \phi_{\text{max}} = 0.62 \text{kV} \) for consistency with EW07 [see also Scudder, 1995] in order to reduce the bulk velocity by about half through the shock (by reducing the bulk
kinetic energy to about one fourth its upstream value, with the potential jump, 
$q\phi_{\text{max}}$, equal to the change in the average kinetic energy). The shock width 
parameter, $\lambda$, is $10^5$ m; this is approximately $\frac{c}{\omega_p}$, consistent with observations 
[e.g., Mellott and Greenstadt, 1984].

The program is looped over values of $S$, $I$, and $\Psi$, with "nshells" shells of 
$S = \text{constant}$ (equally spaced values between 0 and $S_{\text{max}}$); "nlayers" layers of 
$I = \text{constant}$ (between $-S$ and $S$); and "npaths" values of $\Psi$ (between 0 and 
$2\pi$).

For a given set of invariants, we have, from equations (3.74), (3.75), and (3.76):

$$p_1 = B_{ux}\sqrt{S^2 - I^2}\sin(\theta) + B_x I + \dot{m}V_u$$  \hspace{1cm} (3.122)

$$p_2 = |B_u|\sqrt{S^2 - I^2}\cos(\theta)$$  \hspace{1cm} (3.123)

$$p_3 = -B_x\sqrt{S^2 - I^2}\sin(\theta) + B_{ux} I$$  \hspace{1cm} (3.124)

with $\theta = \frac{|B_u|}{\dot{m}V_u B_{ux}} p_2 - \Psi$. Note that $p_2$ is defined implicitly in terms of the 
invariants; in order to determine the values of the phase variables in terms of 
the chosen invariants, we make use of the method of false position. First, the 
momenta are evaluated at $\theta = 0$ and $\theta = 2\pi$, and we calculate $\Psi$ from equation 
(3.71). Then, the method of false position is used to find the value of $\theta$ that 
corresponds to the chosen value of $\Psi$ for the current iteration. Once $\theta$ is known, 
we find the initial momenta values using the above equations.

The particle starts at $x(0) = -2$, $y(0) = 0$, $z(0) = 0$. The particle is then moved 
in time increments of $h = 0.01 s$ using the fourth order Runge-Kutta method 
(RK4) until $x(t)$ is sufficiently large. Test runs at $h = 0.005$ and $h = 0.001$ were 
carried out to verify that the step-size is sufficiently small to give consistent 
results.

While RK4 is sufficient for the present study, we may consider alternatives for 
future work. If the study involves a more narrow shock, an adaptive method
[e.g., Butcher, 2003] - in which the error for each step is estimated by using different order Runge-Kutta methods and the step-size adjusted to control this error - may be necessary to ensure an accurate numerical integration. Another consideration, given the Hamiltonian formulation and the focus on invariants of the flow, is whether the method used preserves the symplecticity of the flow (that is, whether the Poincaré integral invariant, discussed further in Appendix A, is conserved). An example of a symplectic Runge-Kutta method is the Gauss-Legendre Runge-Kutta (GLRK) method [Iserles and Zanna, 1995]. Symplectic Runge-Kutta methods are implicit (and thus more difficult to implement), but may be preferred for further study of the flow invariants.

A normal cubic spline is fit between the points obtained. We then find $t$ such that $x(t)$ takes one of “ntargets” particular values between $-2$ and $10$, and calculate $p_1$, $p_4 = p_2 + Bxz - \alpha(x)$, and $p_3$ at these points using the spline.

### 3.4.1 Shape of the Phase Shell

Figures 3.3-3.9 show the phase shell for different values of $\theta_{bm}$, $S$, and $x$. Except where stated otherwise, we choose an upstream phase shell radius of $|B_u|S = 0.3$. This value is approximately equal to the standard deviation of the phase variables in one direction at $T_u = 10^5K$ ($\sigma = \sqrt{\frac{m k T_u}{q^2}} = 0.2999$, to four significant digits). Note that this is not one standard deviation in the distribution with respect to $S$. Only about 20% of the distribution is within this phase shell, but this is suitable for illustrating the behaviour of the distribution through the shock, as well as calculating the average values of the phase variables.

Upstream (Figure 3.3), the phase shell is spherical as the distribution approaches the shock, and we can see that through the shock (Figure 3.4) the shell initially stretches into an approximately ellipsoidal shape [c.f., EW03]. Downstream, the particles settle into an oscillation in phase space dependent on the downstream gyroradius (Figure 3.5).

The velocity/momentum gyrates about a guiding centre motion. The gyrofrequency, $\Omega_d = \frac{qB}{m}$, is independent of the individual ion velocities - this means that each ion takes the same amount of time to complete one gyroperiod. For a perpendicular shock, the guiding centre motion in the $x$ direction is also the same for all the ions. Therefore, over one gyroperiod all the ions will travel
Figure 3.3: The phase shell corresponding to $|B_u| S = 0.3$ through quasi-perpendicular shock, with $\theta_{bn} = 50^\circ$. Connecting lines are for constant $\Psi$. We also plot, in these and in the following figures, a projection of the phase shell on the $p_1p_4$-plane, in order to clarify the position of the phase shell in the three-dimensional phase space. (top) $x = -0.2$. (bottom) $x = 0$ (midshock).
Figure 3.4: The phase shell corresponding to $|B_u|S = 0.3$ downstream of the shock, with $\theta_{bn} = 50^\circ$. (top) $x = 0.2$. (bottom) $x = 0.4$. 

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Figure 3.5: The phase shell corresponding to $|\mathbf{B}_u|S = 0.3$ downstream of the shock, with $\theta_{bn} = 50^\circ$. (top) $x = 1$. (bottom) $x = 4$. 

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the same distance in \( x \), and phase shell "snapshots" taken at downstream values of \( x \) which differ by a distance corresponding to some integer multiple of a gyroperiod will look the same. The result is the phase space "bunching" of Lee et al. [1986], as the velocity of the downstream distribution oscillates about the Rankine-Hugoniot value [Gedalin, 1996b].

However, this is not the case for a quasi-perpendicular shock [e.g., Gedalin, 1997; Balikhin et al., 2008; Ofman et al., 2009]. Since the ions travel downstream at different guiding centre velocities, the ions toward the faster "end" of the phase shell traverse a smaller portion of their gyroperiod for a fixed distance travelled in the \( x \)-direction than the ions on the slower end of the phase shell. As the figures show, this results in a twisting of the phase shell around the magnetic field lines. Because the individual ion trajectories are restrained to circular paths in phase space, the phase shell is constrained to a toroidal shape, and we can clearly see this torus as we progress downstream. (This is a consequence of the more general result that the trajectories in the 6-dimensional phase space of a Hamiltonian system are along the surface of a static 6-dimensional torus [e.g., Chen and Palmadesso, 1986].)

Figure 3.6 offers two views of the phase shell farther downstream of the shock. From the second perspective, the thin layers of the twisted phase shell can clearly be seen. As the ion population continues downstream, the distance in phase space between these layers decreases, and they become arbitrarily close. As a result, trajectories which are close together downstream may originate from quite different upstream trajectories. In this way, we can see that the system exhibits topological mixing, even in a model in which turbulence from reflected ions or other phenomena is absent [e.g., Percival, 1987; Balikhin et al., 2008; Ofman et al., 2009].

Figure 3.7 compares the shapes of phase shells of different initial radii, with \( |B_0|S = 0.3, 0.6, 0.9, 1.2 \). As we might expect, the twisting effect observed in the previous figures is more rapid for larger values of \( S \).

Note that for sufficiently large values of \( S \), the gyration of some of the ions will result in negative values of \( p_1 \); additionally, some of the ions will initially be unable to overcome the shock potential, resulting in reflection. Here, we only plot the first encounter of a given ion with the plane \( x = 2 \), ignoring any backstreaming ions. For the largest value of \( S \) plotted, this causes an apparent flattening of the phase shell at the phase plane \( p_1 = 0 \). There are no
Figure 3.6: The phase shell corresponding to $|B_u|S = 0.3$ downstream of the shock, with $\theta_{bn} = 50^\circ$. (top) $x = 10$, plotting only data points. (bottom) $x = 10$ from another perspective.
Figure 3.7: The downstream \((x = 2)\) phase shell, with \(\theta_{bn} = 50^\circ\), for different radii: \(|\mathbf{B}_u|S = 0.3\) (top-left); \(|\mathbf{B}_u|S = 0.6\) (top-right); \(|\mathbf{B}_u|S = 0.9\) (bottom-left); \(|\mathbf{B}_u|S = 1.2\) (bottom-right).
backstreaming ions for $|B_u|S = 0.9$, and so we will use this as the limiting shell in our investigation of the temperature.

Figures 3.8 and 3.9 show the phase shell $|B_u|S = 0.3$ for $\theta_{bn} = 65^\circ$ and $\theta_{bn} = 80^\circ$ respectively, at $x = 1$ and $x = 4$. We can see that as the magnetic field orientation approaches fully perpendicular, the phase shell twists about the magnetic field more slowly. (This is because the guiding centre motion in the $x$ direction varies less from one end of the phase shell to the other as the magnetic field is closer to perpendicular.) In the limit of a perpendicular shock, then, the shell would undergo no twisting at all, and instead the shape and position of the shell in phase space would be periodic in $x$, as seen in previous studies [Gedalin, 1996b, EW03].

### 3.4.2 Phase Volume

We now calculate the phase volume at different values of $x$. Because of the twisting that occurs downstream, it is not practical to calculate the volume directly. Instead, we make use of equations (3.99) and (3.100). For each set of initial parameters, the constant $K$ is calculated from the values of the phase variables. We then integrate $K_p$ over the invariants at the different values of $x$ using Romberg's method [Froberg, 1985], with a maximum of 32 intervals for $\Psi$, $I$, and 8 intervals for $S$, with the maximum upstream radius $|B_u|S_{max} = 0.3$; this gives agreement with the known upstream volume ($4\pi(0.3)^3$, the volume of a sphere of radius 0.3) to eight significant digits.

Figures 3.10 and 3.11 show the volumes calculated between $x = -2$ and $x = 10$ for two values of $\theta_{bn}$. Like the shape of the phase shell, the volume is subject to oscillations at two frequencies - one determined by the gyration about the guiding centre, and the other determined by the rate of phase shell twisting due to differences in the guiding centre velocities at the extremes of the phase shell. Downstream, these oscillations are damped, and the volume converges.

Figures 3.12 and 3.13 compare the value of $p_1$ corresponding to the modal ($S = 0$) trajectory, $\bar{p}_1$, and the average value, $p_1^*$, over the phase volume. Through the shock, as the phase shell remains approximately ellipsoidal, the modal and average values are similar. Downstream, the modal value oscillates over a fixed range of values due to gyration (note that this modal value corresponds to an actual physical trajectory, with an upstream velocity equal to
Figure 3.8: The phase shell corresponding to $|B_u|S = 0.3$ downstream of the shock, with $\theta_{bn} = 65^\circ$. (top) $x = 1$. (bottom) $x = 4$. 
Figure 3.9: The phase shell corresponding to $|\mathbf{B}_u|S = 0.3$ downstream of the shock, with $\theta_m = 80^\circ$. (top) $x = 1$. (bottom) $x = 4$. 
Figure 3.10: Volume of the phase shell corresponding to $|B_u|S = 0.3$ with $\theta_0 = 50^\circ$ vs. $x$. 
Figure 3.11: As in Figure 3.10, but with $\theta_{on} = 65^\circ$. 
Figure 3.12: The modal ($p_l^m$, dash) and uniform distribution average ($p_l^u$, solid) values of $p_l$ for trajectories within a phase shell corresponding to $|B_u|S = 0.3$ with $\theta_{in} = 50^\circ$ vs. $x$. 
Figure 3.13: As in Figure 3.12, but with $\theta_{bn} = 65^\circ$. 
the bulk velocity, $V_u$). However, as the phase shell becomes twisted about the magnetic field lines, the gyration of the phase shell as a whole has less effect on the average value, which converges to a value at the centre of the bounding torus. Since, as we have shown above, the volume is inversely proportional to $p_1^*$, the result is the damped oscillation of the volume seen in the previous figures.

The mean value, $\bar{p}_1$, taking into account the probability distribution, is roughly equal to $p_1^*$, and therefore we do not plot it here, though it is used in the calculation of the temperature in the next section. For larger values of $S$, both $\bar{p}_1$ and $p_1^*$ will converge more quickly, but the value they converge to is essentially independent of the choice of $S$.

### 3.4.3 Calculation of the Temperature

Unlike the mean (which is largely independent of $S_{\text{max}}$ sufficiently far downstream) and the volume (which is proportional to $S_{\text{max}}^2$), the variation in the temperature increase through the shock with regards to the phase shell chosen is more complex. Upstream, the variance of a given phase shell, $S = \text{constant}$, is proportional to $S^2$ (since all the trajectories on that shell are at a distance of $|B_u|S$ from the central value, and the variance is the average of the squares of the deviations from the mean). However, through the shock, trajectories which were close together upstream will become spread out as the shell distorts and takes on a toroidal shape, and as a result the relative increase in temperature is much greater for the core of the distribution.

Figure 3.14 illustrates this effect, for $T_u = 10^5K$. We calculate the total temperature (the trace of the temperature tensor) of the distributions contained within two phase shells: $|B_u|S_{\text{max}} = 0.3$, which contains about 20% of the distribution, and $|B_u|S_{\text{max}} = 0.9$, which contains about 97% of the distribution. Upstream, the temperatures of these distributions are approximately $1.88 \times 10^4K$ and $9.19 \times 10^4K$, and the contribution to the temperature of the whole distribution is approximately 3.75% and 89.2% respectively. It is clear from the figure that the ratio of the downstream temperature to the upstream temperature is much higher for the smaller value of $S$. The ratio for the smaller $S_{\text{max}}$ is about 12 and, despite the small initial contribution of the “core” distribution to the total temperature upstream, the downstream temperature converges to a value more than double the upstream temperature of the entire
Figure 3.14: Ion temperature through the shock for the portion of the distribution within the phase shells $|B_u|S_{max} = 0.9$ (solid) and $|B_u|S_{max} = 0.3$ (dash) with $\theta_{bn} = 50^\circ$ vs. $x$. 
distribution. The downstream temperature for the larger value of $S_{\text{max}}$ is about $3.5 \times 10^5$K, but since this larger portion of the distribution started out at a much higher temperature, the downstream to upstream ratio is only about 3.8.

In both cases, we see that the heating is gradual, unlike the situation observed in some low Mach number shocks [e.g., Thomsen et al., 1985] but in agreement with the observations reported by Balikhin et al. [2008] and with computer simulations [e.g., Ofman et al., 2009]. However, note that even for $|B_u|S_{\text{max}} = 0.9$ we are ignoring 3% of the distribution, and we can see that the core of the distribution is slower to converge. Also, amongst the missing tail of the distribution are any backstreaming ions, some of which may contribute more significantly within the early part of the shock ramp before eventually being transmitted after reflection.

Figure 3.15 shows the temperature components for the distribution within the shell $|B_u|S_{\text{max}} = 0.9$. As expected, the temperature is highest in the $y$ direction, which is perpendicular to the magnetic field. Figure 3.16 also plots temperature components, this time parallel and perpendicular to the shock. The downstream to upstream ratio for both perpendicular components converges to around 5, while the parallel component of the temperature only increases by about 50%.

Figures 3.17-3.18 show the total temperature, along with the parallel and perpendicular temperature components, for different values of $\theta_{bn}$ (65°, 80°). There are three important features we can see in these plots as compared to Figures 3.14 and 3.16. First, total heating is greater for higher values of $\theta_{bn}$. Whereas the downstream to upstream temperature ratio is 3.8 for $\theta_{bn} = 50^\circ$ (within the phase shell $|B_u|S_{\text{max}} = 0.9$), the ratio is around 4.2 for $\theta_{bn} = 65^\circ$ and about 4.5 for $\theta_{bn} = 80^\circ$.

Second, the degree to which the downstream temperature is anisotropic increases as the magnetic field approaches a perpendicular orientation: heating parallel to the magnetic field is less significant for $\theta_{bn} = 65^\circ$, and almost non-existent for $\theta_{bn} = 80^\circ$ [c.f., Wilkinson, 1995]. The ratio $\frac{T_{\parallel}}{T_{\perp}}$ is between 3.2 (50°) and 6.1 (80°), which is in agreement with the observations of the AMPTE/IRM spacecraft, with Sckopke et al. [1990] showing a ratio in the core of the distribution greater than 3 and as high as 7, as shown in Figure 3.19 (note the jumps observed in the ion temperature perpendicular to the magnetic field in panel five). The magnitudes of these ratios are also in agreement with
Figure 3.15: Temperature components in the $x$ (solid), $y$ (long dash), and $z$ (short dash) directions for the distribution within the shell $|B_u| S_{max} = 0.9$ with $\theta_{bn} = 50^\circ$ vs. $x$. 
Figure 3.16: Temperature components in the $b$ (parallel to the magnetic field, solid), $y$ (long dash), and $k$ (perpendicular to the magnetic field in the $xz$-plane, short dash) directions for the distribution within the shell $|\mathbf{B}_u|S_{max} = 0.9$ with $\theta_{bn} = 50^\circ$ vs. $x$. 

\[ T_k \times 10^5 \text{ (K)} \]
Figure 3.17: The total temperature (solid) and temperature components in the $b$ (long dash), $y$ (short dash), and $k$ (dotted) directions for the distribution within the shell $|B_u|S_{max} = 0.9$ with $\theta_{bn} = 65^\circ$ vs. $x$. 
Figure 3.18: As with Figure 3.17, but for $\theta_{on} = 80^\circ$. 
Figure 3.19: AMPTE/IRM measurements for September 5, 1984 shock crossings with $\theta_{\text{on}} = 73^\circ$ for the first interval (between crossings into and out of the magnetosheath at 0348 and 0406 UT respectively) and $\theta_{\text{on}} = 73^\circ - 80^\circ$ for the second (crossings at 0410 and 0445 UT). From top to bottom: Magnetic field magnitude, in nT; Plasma density, in cm$^{-3}$; Plasma bulk speed in km/s; Electron temperature in units of 10$^6$K; Ion temperature perpendicular and parallel to the magnetic field in units of 10$^6$K; Ion temperature anisotropy; Power of magnetic fluctuations in the frequency range 0.3 – 0.8$\omega$ci. From Sckopke et al. [1990].
the findings of Thomsen et al. [1985] for a sample of ten quasi-perpendicular shocks (Figure 3.20).

Third, because the twisting of the phase shell occurs more slowly for a more perpendicular shock, as seen in earlier figures, it takes longer for the distribution to spread out in phase space, which means that heating of the core distribution is less rapid as $\theta_{bn}$ approaches 90°, in agreement with the analysis of Ofman et al. [2009]. As with the $\theta_{bn} = 50°$ case, these plots ignore a portion of distribution, and including the outlying portion and the reflected ion distribution may mitigate the apparent departure from the rapid heating found in some space observations. Of course, it is also possible that instabilities, not considered in this model, play a role in the rapid heating through these shocks as suggested by, e.g., Thomsen et al. [1985], Winske [1985b], and references therein.

3.5 Summary and Conclusions

In this chapter, the problem of the heating of directly transmitted ions through a collisionless shock has been examined from a statistical mechanics viewpoint, generalizing the results of EW03 to a three-dimensional phase space for a quasi-perpendicular shock model. Unlike the study of EW07, which considers surfaces of constant energy, we analyze the properties of phase shells which are surfaces of constant probability. These phase shells are initially spherical upstream of the shock as the ion distribution is Maxwellian (isotropic), but through the shock the shells distort due to the uneven deceleration of the ions as well as the unequal gyratory motion of ions at different locations in the phase space.

A Hamiltonian formulation of the ion mechanics has been developed which is linear in $y$, allowing for the simplification of Liouville's equation which has been used to study the evolution of the distribution through the shock. The general solution to Liouville's equation is found as a function of several invariants; one of these is the Hamiltonian itself, but as the Hamiltonian depends on $y$ whereas the initially Maxwellian upstream distribution depends only on the velocity of the ion, we have not used the standard statistical physics model, instead expressing the probability distribution in terms of the invariant $S$. This invariant is the three-dimensional generalization of the invariant used in EW03.
Figure 3.20: Temperature ratios across ten quasi-perpendicular shocks observed by ISEE. Ion/electron temperature ratios are represented by circles/triangles; perpendicular/parallel ratios are filled/unfilled. From Thomsen et al. [1985].
for perpendicular shocks, though for quasi-perpendicular shocks the upstream form of $S$ is not equated with the upstream ion gyroradius.

In addition to assumptions of planarity and steady state fields, the noncoplanar component of the magnetic field has been ignored through the shock. Theoretical estimates of the size of the noncoplanar magnetic field have been obtained by Jones and Ellison [1987] and Gedalin [1996a]. The former study assumes that the ion contribution to the total current in the shock ramp is negligible compared to the electron contribution and its predictions are in good agreement with measurements at low Mach number shocks [Friedman et al., 1990]. At higher Mach numbers, the presence of reflected ions renders the above assumption invalid and the predicted values significantly underestimate the integrated value of the noncoplanar component [Gosling et al., 1988; Friedman et al., 1990]. Gedalin [1996a] obtains general expressions for the noncoplanar component of the magnetic field from two-fluid hydrodynamic equations under the assumptions of stationarity, one-dimensionality and quasi-neutrality of the shock. These expressions highlight the contribution of the electron pressure anisotropy and the off-diagonal component of the ion pressure (see also Gedalin and Zilbersher [1995]) which arises when reflected ions are present [Gedalin, 1996a].

The role of the noncoplanar component of the magnetic field in the deceleration of the ions is particularly important in the de Hoffman-Teller frame of reference [Thomsen et al., 1987; Gedalin and Balikhin, 2004]. In the Normal Incidence frame used in our current study, the magnetic deceleration due to the noncoplanar component of the magnetic field is unimportant, as noted by Gedalin and Balikhin [2004], particularly when one takes into account the small ramp widths (of the order of $\frac{v}{\omega_{pi}}$ [Mellott and Greenstadt, 1984; Farris et al., 1993]) typical of low Mach number shocks and used in the current study (see section 5). Moreover, the noncoplanar magnetic field is observed to be tiny at weak low Mach number shocks [Balikhin et al., 2008] and is therefore often neglected in theoretical analyses of the ion behavior at low Mach number perpendicular and quasi-perpendicular shocks [e.g., EW03; Ofman et al., 2009].

Through a coordinate transformation from the canonical momenta (velocity space) to an invariant space (using $S$, along with two other invariants, $I$ and $\Psi$), an expression has been derived for the volume of phase shells of constant probability (related to the temperature of the distribution), which has been found to be inversely proportional to the average value of the momentum in the
shock normal direction \((p_1)\) within the volume. This result is a generalization of the result of EW03, where the limit of the phase volume as \(S\) approaches zero is shown to be inversely proportional to the modal value of \(p_1\).

One key feature found in the heating of directly transmitted ions is that the mean and mode of the distribution are not the same, as discussed in EW06 where it is shown that a separation in the mean and mode is necessary for heating to take place. For a perpendicular \((\theta_{bn}=90^\circ)\) shock, both the mode and mean oscillate downstream of the shock, as the entire distribution gyrates about the magnetic field. However, we find that for a quasi-perpendicular shock, the mean converges to the Rankine-Hugoniot value far downstream. Physically, this is explained by noting that the guiding center velocity of an ion is dependent on the location in phase space (whereas for a perpendicular shock, all ions have the same guiding center velocity), while the gyrofrequency is constant (far enough downstream to assume \(B = B_d = \text{constant}\)). This results in a “twisting” of the phase shell; while the gyroperiod of each ion is the same regardless of its location in the phase space, the distance traveled in that time depends on the guiding center motion, and thus ions which have traversed the same distance normal to the shock do not complete the same number of gyrations about the magnetic field. Because of this twisting, the phase space distribution is spread more evenly about the central Rankine-Hugoniot value, and the mean converges (while the modal trajectory continues to oscillate).

The heating through low Mach number shocks has been the focus of previous studies, including Gedalin [1996b, 1997]; EW06; and Ofman et al. [2009]. In some of these studies, thermalization is explained by noting that a jump in the electrical potential energy (equivalently, a decrease in the kinetic energy) results in an unequal decrease in the velocities of ions, since the kinetic energy is quadratic with velocity. Thus, the spread in energies remains the same for an abrupt potential change, but the spread in velocities changes. Like the distribution mean, the temperature converges far downstream for a quasi-perpendicular shock. The heating is seen to be anisotropic, in agreement with observational studies [Thomsen et al., 1985; Sckopke et al., 1990]. Physically, this is again explained by the gyration about the magnetic field, as seen in Gedalin [1996b, 1997]; EW03; and Ofman et al. [2009].

The shape and volume of constant probability phase shells have also been studied, along with other distribution properties such as the mean velocities and the temperature, using numerical methods. Unlike a perpendicular shock, the
phase shell does not adopt an approximately Gaussian form downstream, but instead twists around field lines as a result of unequal guiding center motion. Because of this, the mean velocity/momentum and temperature converge far downstream, rather than oscillating about the Rankine-Hugoniot values, consistent with the observations reported by Balikhin et al. [2008] and the analytical studies of Gedalin [1997] and Ofman et al. [2009]. The heating profile does not match the rapid heating observed in space [e.g., Thomsen et al., 1985; Sckopke et al., 1990], but we expect this is in part due to ignoring the tails of the distribution as well as the possible contribution of some reflected-gyrating ions. The core of the distribution is slower to twist and spread in phase space, and therefore heating of the core is less rapid.
Chapter 4

Concluding Remarks

Two problems regarding the thermalization of the ion distribution at collisionless shocks have been considered in this thesis. This chapter summarizes the results of the investigations and examines potential areas for future research in these topics.

The trajectories of ions specularly reflected from curved collisionless shocks have been studied. The primary parameter for determining the end result of a given particle's reflection is the angle between the magnetic field and the shock normal, $\theta_{bn}$. The precise boundaries between not returning, returning, and returning with increased normal velocity depend on two other factors - the curvature of the shock at reflection relative to the ion gyroradius, and the angle of incidence - which both vary with the shape of the shock. Planar, cylindrical, spherical, and parabolic shock geometries have been considered. The incident normal velocity of the individual ions relative to the bulk velocity also becomes an important factor for higher temperatures.

This work could be expanded to look at other shock geometries. Elliptical or hyperbolic curves may more closely approximate the true shape of the bow shock. These geometries could be studied with a methodology similar to that used here to study the parabolic geometry, though the calculation of the distance between the ion and the shock requires solving a quartic equation rather than a cubic.

The model may also be used to revisit other work on planar shocks. For example, if a particle returns to the shock with a smaller normal velocity, it will be reflected again, while an ion reflected from a quasi-perpendicular shock may
reencounter the shock with an increased normal velocity, yet still lack sufficient energy to overcome the shock potential (see Figure 2.16). Thus, a particle could reflect from the shock many times before overcoming the potential barrier or escaping upstream [Wilkinson, 1999]. In order to model this, we can simply calculate $t$ such that the particle reencounters the shock, and then use the values of $r(t)$ and $v(t)$ as the new $r_i$ and $v_i$ respectively for another iteration.

For curved shocks, ions undergoing multiple reflections will see a different magnetic field orientation relative to the shock normal ($\theta_{bn}$) at every reencounter. The motion along the shock front of an ion initially reflecting in the quasi-parallel region of the shock might carry it into the quasi-perpendicular region before it can escape upstream, allowing an increase in normal velocity (and eventual transmission through the shock) after subsequent reflection. Conversely, an ion reflecting in the quasi-perpendicular regime might experience an increase in normal velocity after its first reflection(s) but eventually escape upstream if its motion carries it into the quasi-parallel regime.

Another possible topic of future work involves the non-specular reflection of ions. While specular reflection is a good assumption for a smooth, narrow shock, variations in the shock potential and magnetic field (particularly in the turbulent quasi-parallel region of the shock), as well as gyration within a non-zero width shock ramp, will lead to variation in the outgoing distribution. Sckopke et al. [1983] incorporates this into a planar model by assuming that some portion of the reflected distribution is reflected non-specularly so that they are emitted isotropically into the entire upstream hemisphere. An alternative would be to use a model of the magnetic field and shock potential that changes gradually over a finite shock width, such as that used in Chapter 3, adapting the model to a curved shock geometry.

The effect of shock reformation on the trajectories of reflected ions is a further area of interest. While a quasi-stationary shock serves as a good model for studying the effects of curvature on the parameters necessary for ions to return to the shock front (as compared to planar quasi-stationary results), for sufficiently high Mach number, high $\theta_{bn}$ shocks, shock reformation may result in changes in the magnetic field on the ion gyroperiod time scale, affecting the results presented. It may be possible to study the effects of self-reformation on ion reflection at curved shocks analytically using an appropriate periodic field/potential model, or numerically using existing simulation techniques.

The second area of research presented in the thesis involves the thermalization
of the transmitted ion distribution at low Mach number, quasi-perpendicular shocks. A Hamiltonian formulation has been used, and the evolution of the phase volume, average trajectories, and temperature of an initially Maxwellian distribution has been studied analytically. These results have been further investigated using numerical calculations, with a simple model for the magnetic field and electrostatic potential through the shock. Phase shells of constant probability (initially spherical) are found to distort, twisting about the magnetic field as a result of out-of-phase oscillations, in contrast to the periodic changes found in previous work on perpendicular shocks. The effect of the magnetic field orientation on the shape and volume of these phase shells as well as the temperature of the distribution has also been considered, and we find in each case that the temperature exhibits a $T_\perp > T_\parallel$ anisotropy, in agreement with previous observations and theoretical studies.

In the planar model considered in this thesis, a number of extensions might be considered. The tails of the distribution (including any initially reflected ions) have been ignored in the present study, but these outliers may be key in explaining the rapid heating through the shock ramp found in observational results. The effect of different shock widths on the thermalization of the ions can be investigated by varying the shock width parameter, $\lambda$. In EW03, the authors note that for a perpendicular shock, maximum anisotropic heating occurs in the zero shock width case, while stretching occurs more uniformly for a wide shock, with the phase shell remaining approximately circular.

The work in Chapter 3 has also assumed fixed fields and a steady state solution to Liouville's equation, yet, in reality, the fields and solar wind conditions are variable and the fields depend on the positions and velocities of the ions (and electrons). Hybrid and full-particle simulations would allow for the self-consistent calculation of the fields in a numerical setting, though the inclusion of self-consistent fields in a Hamiltonian formulation may be analytically intractable. Chapman [1994] investigates magnetic reversal in current sheets with a parabolic field model. In a static model, the form of the Hamiltonian used is similar to that used in Chapter 3 of the present thesis, and the author finds that while in a static model the ion trajectories are fixed in regimes of either regular or stochastic behaviour, they are able to transition between regimes in a time-dependent model. This paper might serve as a starting point for the study of transmitted ion trajectories at shocks with time dependence.
Above, a model for studying the non-specular reflection of ions at curved shocks is suggested, and such a model might also be used to study the transmitted distribution at low Mach number shocks for curved shocks. An obvious complication in this case would be that the distribution is no longer independent of $y$ and $z$, and so a change to a cylindrical or spherical polar coordinate system might be more appropriate.

EW03 note that a stronger result than that given by equation (3.106) holds in the perpendicular (two-dimensional) case. For any measurable region, $R$, of the $p_1 > 0, p_2$ halfspace:

$$\int_R p_1 dp_1 dp_2 = \text{constant} \quad (4.1)$$

This result is derived from the Poincaré-Cartan integral invariant in Appendix A. An additional goal of future work may be to generalize this result to a quasi-perpendicular (three-dimensional) shock.

A key concept in the thesis is that of anisotropic, kinetic thermalization through the bow shock. In Chapter 2, an effective dissipation is achieved through the reflection of a portion of the ion distribution, separating the distribution into two or more phase space populations. In Chapter 3, the non-linear relationship between the kinetic energy of the ions and their velocity results in a non-uniform slowing of different portions of the distribution, and thermalization occurs preferentially perpendicular to the magnetic field as the ions gyrate downstream of the shock. In both cases, we have mentioned that “true” thermalization results in Maxwellian distributions, and some downstream process must be responsible for this. A possible extension of the work presented in both studies could be an investigation of the interaction between the ion distributions calculated downstream of laminar or supercritical shocks with the instabilities mentioned in the literature as possible downstream thermalization mechanisms, comparing the theoretical heating from these instabilities applied to our analytically derived distribution to the observed heating patterns in the literature.

Downstream of the low-Beta, low Mach number shock crossings studied by Sckopke et al. [1990], referenced above in relation to the temperature anisotropy, the low frequency wave activity is dominated by left-hand polarized
waves (both in the spacecraft frame and in frame moving with the transmitted ions). The spectra peak in the frequency range between 0.3 and 0.8 times the proton cyclotron frequency and sometimes display a double-hump. In order to understand these features, Brinca et al. [1990] conducted a linear wave stability analysis of the state downstream of these shocks. This was modeled as a background hydrogen magnetoplasma with an anisotropic (\(T_{\parallel} > T_{\perp}\)) transmitted ion population permeated by a hotter dilute beam of anisotropic protons representing the population of ions originally reflected at the shock. This study reproduces the above basic features of the observed wave activity. The double-humped structure of the spectra arises from the two free energy sources in the model: the anisotropic transmitted ions destabilize the electromagnetic left-hand ion cyclotron instability just below the proton cyclotron frequency and the beam ions feed the same mode at lower frequencies. The authors point out that their analysis, which assumes gyrotropic ion velocity distributions, is unlikely to apply to measurements just downstream of the shock and that a more detailed interpretation of the observed turbulence would require consideration of the nonlinear evolution of the instabilities and of the self-consistent interaction between the particles and the waves.

Liu et al. [2005] have developed a quasilinear model to predict the quasi-equilibrium bulk ion and wave parameters sufficiently far downstream of the shock, ignoring timescales larger than that of the Alfven ion cyclotron instability and assuming that the fluctuation power of the waves is small. The authors model the reflected and transmitted ion populations separately, as the waves excited by each do not affect the distribution of the other. The inclusion of the core ion distribution for a perpendicular shock reproduces the double-humped power spectrum seen in Brinca et al. [1990], finding that dispersive effects are important in matching the observations of Sckopke et al. [1990]. Their analysis of the core ion distribution downstream of the shock assumes a negligible shock width, such that the distribution is modified through the shock only by the loss of kinetic energy in the normal direction corresponding to the potential jump, and additionally the authors assume the both the reflected and transmitted distributions are gyrotropic, using a spatially averaged distribution function. In contrast, the present study models the temperature anisotropy of the transmitted ions while preserving the coherence of the ion motion far downstream of the shock for quasi-perpendicular magnetic field geometries, and an application of the resulting non-gyrotropic distribution to the quasilinear model of Liu et al. [2005] may be of interest.
Appendix A

Poincaré Invariants

In Chapter 1, we showed that the magnetic moment of a charged particle's motion through slowly changing fields is approximately invariant. We now relate this approximate invariant to the more general Poincaré invariant:

\[ I = \int_{C(t)} p \cdot dq \]  

(A.1)

where \( C(t) \) is a closed curve. The invariance of this integral results from the property that the phase space of a Hamiltonian system is a symplectic manifold.

For an individual particle, this invariant would seem to only be of interest if the closed curve, \( C \), corresponds to the particle's trajectory. From Section 1.1.2, we have one example of such a periodic particle trajectory: the perpendicular motion of a charged particle in the presence of a constant, homogeneous magnetic field and no electric field is circular. However, for more complicated field profiles, we require an approximation to the Poincaré invariant since, due to drift motion or motion parallel to the magnetic field, an ion's trajectory may not close.

The action integrals, \( J_i \), are term-by-term approximations of the Poincaré invariant:

\[ J_i = \int_{C} p_i dq_i \]  

(A.2)
where the integral is evaluated over one cycle of the oscillation of a periodic generalized coordinate, \( q_i \). The action integral is invariant for slow changes to the system [e.g., Northrop, 1963] - that is, the action integrals are adiabatic invariants, the first of which is the magnetic moment.

Since there are three spatial degrees of freedom, there are three different action integrals, and thus three adiabatic invariants corresponding to different types of motion. The magnetic moment corresponds to the gyration of the particle over a Larmor orbit. The longitudinal invariant relates to motion along the magnetic field lines; as discussed in Section 1.1.3, the invariance of the magnetic moment results in magnetic mirrors, as a sufficiently strong magnetic field slows and reverses the velocity parallel to the field. Thus, the longitudinal invariant is:

\[
\mathcal{J} = \int v_\parallel ds
\]

where \( s \) is along the guiding centre motion [Parks, 2003]. This integral is evaluated over "bounces" between magnetic mirror fields. The third action integral, the flux invariant, is associated with the drift velocity. This invariant is less commonly used, because of the relatively long periodicity of the drift motion [Boyd and Sanderson, 2003].

The Poincaré invariant can be generalized for a time-dependent Hamiltonian by the addition of a term, resulting in the Poincaré-Cartan integral invariant:

\[
\mathcal{I} = \int p dq - \mathcal{H} dt
\]

We can relate the result of equation (4.1) to this invariant. In the EW03 model, we have a Hamiltonian:

\[
\mathcal{H} = \frac{1}{2m} \left( p_1^2 + (p_2^2 - \alpha(x))^2 \right) + \phi(x) - V_0 B_{0y}
\]

with flow invariant \( S \). We wish to write the area \( \Delta \) bounded by the intersection of \( S = \text{constant} \) with \( x = \text{constant} \) in terms of the first Poincaré-Cartan integral invariant:
\[
\int_{C_1} \mathbf{p} \mathbf{d}q - \mathcal{H} \mathbf{d}t = \int_{C_2} \mathbf{p} \mathbf{d}q - \mathcal{H} \mathbf{d}t \quad (A.6)
\]

where $C_1$ and $C_2$ are closed curves in phase space around the same "tube" of trajectories. Since $x$ is constant, we can eliminate the $\mathbf{d}x$ term. Also, note that for this flow, $\mathbf{d}p_2 = V_u \mathbf{B}_u \mathbf{d}t$ (since the Hamiltonian is linear in $y$), and:

\[
\int_C p_2 \mathbf{d}y = - \int_C y \mathbf{d}p_2 \quad (A.7)
\]

We are left with the invariant:

\[
-\frac{1}{V_u \mathbf{b}_u} \int_{C(x)} \frac{1}{2m} \left( p_1^2 + (p_2 - \alpha(x))^2 \right) + \phi(x) \mathbf{d}p_2 = \text{constant} \quad (A.8)
\]

where $C(x)$ is a closed curve of constant $x$. Along this curve, $\phi$ and $\alpha$ (functions of $x$) are also constant. Additionally, the $p_2$ terms vanish for integration around a closed curve, so we are left with:

\[
\int_{C(x)} p_1^2 \mathbf{d}p_2 = \text{constant} \quad (A.9)
\]

and equation (4.1) follows by Green's Theorem. Therefore, the area of $R$ (in particular, for $R = \Delta$, the area of the phase shell $S = \text{constant}$) is inversely proportional to some intermediate value of $p_1$. 

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Appendix B

Simulation Algorithms

In Chapter 1, we discussed one example of a simulation algorithm, the hybrid method of Winske [1985a]. In this appendix, we discuss alternative simulation methods, both hybrid and full-particle, in order to better understand how they incorporate the mechanics described in the Lorentz equation and Maxwell’s equations, as well as highlighting results which relate to the present thesis.

B.1 Vlasov-Fluid Formulation

Quest [1989] reviews the (hybrid) Vlasov-fluid formulation, which combines aspects of MHD and kinetic theory. Here, the electrons are treated as a massless fluid (with the same overall charge as the ion population; with the assumption that the only ions present are protons, this gives \( n_e = n_i = n \)), while the ion dynamics come from the Vlasov equation, which for a collisionless plasma is:

\[
\left( \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla + \mathbf{a} \cdot \nabla_{\mathbf{v}} \right) F_i = 0 \quad (B.1)
\]

where \( F_i \) is the ion distribution function. The second moment of this equation is the ion momentum equation:

\[
m_i n \frac{d\mathbf{V}_i}{dt} = -\nabla \cdot \mathbf{P}_i + n \left( \mathbf{E} + \frac{\mathbf{V}_i \times \mathbf{B}}{c} \right) \quad (B.2)
\]
where $V_i$ is the bulk ion velocity. The electron momentum equation used is:

$$0 = -\nabla P_e - n \left( E + \frac{V_e \times B}{c} \right)$$  

(B.3)

where the left hand side is 0 due to the assumption that the electrons are massless. Combining these momentum equations gives:

$$m_e n \frac{dV_i}{dt} = -\nabla \cdot P_i - \nabla P_e + \frac{J \times B}{c}$$  

(B.4)

Completing the equations for the Vlasov-fluid method are Faraday's and Ampere's laws, along with a polytropic equation of state ($PV^\gamma = \text{constant}$).

### B.2 Full-Particle Code

Hybrid simulations necessarily ignore any kinetic effects due to the electrons. In contrast, full-particle codes treat both the ion and electron species kinetically. In an explicit algorithm, the fields are calculated in a “leap-frog” manner, with the particle velocities calculated at half time-steps from the previous time-step’s fields, and then the fields for the next time-step calculated using these velocities [Mason, 1981]. However, explicit algorithms often require spatial and time scales which are much smaller than the phenomena being studied. As the algorithms are stiff [Quest, 1989], the stability of the code depends on the size of the cells and time-steps used via the Courant condition:

$$\max [\omega_p] \Delta t < 2$$  

(B.5)

where $\omega_p$ is the relevant plasma frequency. In order to include electron kinetic effects, then, either more computational power is required due to the small mass of the electrons compared to the ions, or a different method is needed to avoid the stability constraint.
B.2.1 Implicit Fields

Mason [1981] uses an implicit electric field to avoid this constraint. First, the velocity evolution equation (Lorentz force) is replaced by an averaging:

$$J^{m+\frac{1}{2}} = J^{m-\frac{1}{2}} + \frac{1}{m_\alpha} \left[ \frac{\partial \mathcal{P}}{\partial x} - q n^m E^* \right]$$  \hspace{1cm} (B.6)

where $\mathcal{P}$ is the pressure tensor, $E^*$ is the implicit electric field, and $\alpha$ denotes the particle species. (Here, and throughout this appendix, we use superscripts to denote the time-step.) Note that this takes a similar form to the equation of motion for a fluid element in MHD [c.f., equation (1.35)]. Similarly, a continuity equation is used for the particles, and a predicted electric field can be calculated from Poisson’s equation:

$$E^{m+1} = 4\pi \int_0^x \sum_\alpha q_\alpha n_\alpha^{m+1} dx + E^{m+1}(0)$$  \hspace{1cm} (B.7)

In both of these equations, the quantities calculated are predictions, not necessarily equal to the quantities that will be calculated in the next cycle. The author notes that $E^{m+1}$ is the simplest and most stable choice for $E^*$, but instead uses:

$$E^* = \theta E_i + (1 - \theta) E_c$$  \hspace{1cm} (B.8)

where $\theta \in [0, 1]$ is introduced for flexibility, $E_c = \frac{1}{4} [E^{m+1} + 2E^m + E^{m-1}]$, and $E_i = E^{m+1}$ is the fully implicit field. The predicted field, $E^*$, can then be used to advance the particles.

Brackbill and Forslund [1982] give an implicit derivation in two dimensions, with the full set of Maxwell’s equations:

$$\frac{1}{c} (B^{n+1} - B^n) + (\nabla \times E^{n+\theta}) \Delta t = 0$$  \hspace{1cm} (B.9)
\[ \nabla \cdot \mathbf{B}^n = 0 \quad \text{(B.10)} \]

\[ \frac{1}{c}(E^{n+1} - E^n) - (\nabla \times \mathbf{B}^{n+\theta}) \Delta t = -\frac{1}{c} 4\pi J^{n+\Gamma} \Delta t \quad \text{(B.11)} \]

\[ \nabla \cdot E^{n+\theta} = 4\pi N^{n+\theta} \quad \text{(B.12)} \]

\[ x_{sp}^{n+1} - x_{sp}^n = u_{sp}^{n+\theta} \Delta t \quad \text{(B.13)} \]

\[ u_{sp}^{n+1} - u_{sp}^n = \frac{q_s}{m_s} \left( E^{n+\theta} + \frac{u_{sp}^{n+\Gamma} \times \mathbf{B}^n}{c} \right) \Delta t \quad \text{(B.14)} \]

where the time steps \( n + \theta \) and \( n + \Gamma \) are calculated as interpolates from the values at \( n \) and \( n + 1 \). To advance the fields, \( N^{n+\theta} \) and \( J^{n+\Gamma} \) are needed. Rather than estimating these as moments of the Vlasov equation, as Mason does, Brackbill and Forslund instead start with the definitions:

\[ N^{n+\theta}_s = q_s \sum_p h(x - x_{sp}^{n+\theta}) \quad \text{(B.15)} \]

\[ J^{n+\Gamma}_s = q_s \sum_p u_{sp}^{n+\Gamma} h(x - x_{sp}^{n+\Gamma}) \quad \text{(B.16)} \]

where \( h \) is a shape factor. In equation (B.15), \( h \) is expanded about \( x_{sp}^{n+\theta} \) using (B.13) to yield:

\[ N^{n+\theta}_s = q_s \sum_p h(x - x_{sp}^n) - (u_{sp}^{n+\Gamma} \theta \Delta t) \cdot \nabla h|_{x=x_{sp}} + \cdots \]

\[ = N^n_s - \nabla \cdot J^{n+\Gamma} \theta \Delta t \quad \text{(B.17)} \]
Equation (B.16) is likewise expanded, first by substituting the Lorentz force (B.14):

\[
J_s^{n+\Gamma} = q_s \sum p u_{sp} h(x - x_{s_{sp}}^{n+\Gamma}) + \frac{q_s^2}{m_s} \sum \left( E^{n+\theta} + \frac{u_{sp}^{n+\Gamma} \times B^n}{c} \right) (\Gamma \Delta t) h(x - x_{s_{sp}}^{n+\Gamma})
\]

and, in the limit of no spatial discretization, this becomes:

\[
J_s^{n+\Gamma} = J_s^n - \frac{\nabla \cdot J_s^n J_s^{n+\Gamma}}{N_s^n} + \frac{q_s}{m_s} \left[ \frac{\nabla^{n+\theta} E^n + J_s^{n+\Gamma} \times B^n}{c} \right] (\Gamma \Delta t) q_s \nabla \cdot \hat{P}_s
\]

where \(\hat{P}_s\) is the plasma pressure tensor:

\[
\hat{P}_s = \sum p u_{sp}^{n} u_{sp}^{n+\Gamma} h(x - x_{s_{sp}}^{n})
\]

and \(\hat{u}\) is the fluctuating velocity (variation from the mean velocity).

Further moments could be determined in a similar way, but the authors obtain the pressure evolution without an energy equation. Several options for approximating the pressure are offered. For a cold plasma, \(\hat{P}_s = 0\). This is a stable assumption for \((k\lambda_D)^2 < 1\). If, instead, \((k\lambda_D)^2 = O(1)\), the pressure can be approximated from the particle data, \(\hat{P}_s = P_s^n\), but this adds a stability limit, \(k_s c_s \Delta t < 2\pi\) (when \(\theta = \Gamma = \frac{1}{2}\))

In order to avoid this limit, an implicit formulation can once again be used instead, with the pressure tensor split into a scalar pressure \((\nabla \cdot \nabla) P_s^n = \nabla \cdot (\nabla \cdot \hat{P}_s^n)\) and a residual \(\hat{Q}_s^n = \hat{P}_s^n - P_s^n I\). With a temperature obtained from \(I_s^n = n_s^n kT_s^n\), the scalar pressure is then advanced as:

\[
P_s^{n+\theta} = n_s^{n+\theta} kT_s^n.
\]

The algorithm for the code ("VENUS") is in terms of the scalar and vector potentials, where:
\[ E = -\nabla \phi - \frac{1}{c} \frac{\partial A}{\partial t} \quad (B.21) \]

\[ B = \nabla \times A \quad (B.22) \]

As an additional constraint on \( A \), the authors choose the Coulomb gauge:

\[ \nabla \cdot A = 0 \quad (B.23) \]

Then, in difference form, the equations to be solved are:

\[
-\frac{1}{c^2} \frac{A^{n+1} - 2A^{n} + A^{n-1}}{\Delta t^2} + \nabla^2 A^{n+\theta} = \frac{-4\pi J^{n+\Gamma}}{c} \\
+ \frac{1}{c} \frac{\nabla \phi^{n+1} - \nabla \phi^{n}}{\Delta t} \quad (B.24)
\]

and:

\[ -\nabla^2 \phi^{n+1} = 4\pi N^{n+1} \quad (B.25) \]

along with (B.17) and (B.19).

**B.2.2 Fluctuations and the Massless Electron Assumption**

Note that the appearance of a pressure term as a product of fluctuations in the previous section is similar to the term obtained by assuming a massless species and averaging over the particles, such as is used for the electrons in the hybrid code of Winske [1985a] discussed in Section 1.1.6. For example, consider the Lorentz force acting on a single (massless) particle, \( k \); the force must be 0, so:
0 = q(E_k + u_k \times B_k)

⇒ E_k = -u_k \times B_k \quad (B.26)

where E_k and B_k are the fields at the particle’s location. Letting \( \bar{u} \) be the mean velocity over the collection of particles and with u_k representing a velocity fluctuation as above (and similar notation for the fields), we have:

\[
E_k = -(\bar{u} + u_k) \times (\bar{B} + B_k) \quad (B.27)
\]

\[
E_k = - (\bar{u} \times \bar{B} + u_k \times \bar{B} + \bar{u} \times B_k + u_k \times B_k) \quad (B.28)
\]

Averaging over the particles, the first term is constant (and drops out of the sum) while the middle two terms vanish (as the average of the fluctuations is zero - this property is preserved by the cross product, a linear operator), so:

\[
\bar{E} = -\bar{u} \times \bar{B} - \frac{\sum_k u_k \times B_k'}{n} \quad (B.29)
\]

For small fluctuations in one dimension, we can write B_k' as \( \frac{\partial B}{\partial z} \tilde{x}_k \), giving the expression:

\[
\bar{E} = -\bar{u} \times \bar{B} - \frac{\sum_k \tilde{x}_k u_k \times \frac{\partial B}{\partial z}}{n} \quad (B.30)
\]

### B.3 Noise Properties and Selected Simulation Studies

Langdon [1972] compares several full-particle algorithms and their noise properties, finding that, while methods using the potentials (A and \( \phi \)) show less noise than those using the fields (E and B) [Morse and Nielson, 1971], this is
due to differences in the calculation of the current density from the particle data rather than the choice of potentials over fields.

The equations given for the potential-based method are:

\[ \nabla^2 A - \frac{1}{c^2} \frac{\partial^2 A}{\partial t^2} = \frac{4\pi}{c} \]  
(B.31)

\[ \mathbf{J}_t = -\frac{4\pi}{c} (\mathbf{J} - \nabla \zeta) \]  
(B.32)

\[ \nabla^2 \phi = 4\pi \rho \]  
(B.33)

\[ \nabla \cdot \mathbf{A} = 0 \]  
(B.34)

\[ \nabla^2 \zeta = \nabla \cdot \mathbf{J} \]  
(B.35)

where \( \nabla \) and \( \frac{\partial}{\partial t} \) represent difference operators in the code, \( \rho \) and \( \mathbf{J} \) are calculated by distributing charge and current density from each particle to the nearest grid points, and \( \zeta = \frac{\partial \phi}{\partial t} \). The author finds that these equations result in the same field equations as using the fields directly, except that the current and charge densities do not satisfy the continuity equation. Thus, the author instead uses:

\[ \nabla \times \mathbf{E} + \frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} = 0 \]  
(B.36)

\[ \nabla \times \mathbf{B} - \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} = \frac{4\pi}{c} \mathbf{J}' \]
\[ \equiv \frac{4\pi}{c} (\mathbf{J} - \nabla \zeta) \]  
(B.37)
with:

$$\xi \equiv \zeta - \frac{1}{4\pi} \frac{\partial \phi}{\partial t} \quad (B.38)$$

where \( \xi \) satisfies:

$$\nabla^2 \xi = \nabla \cdot J + \frac{\partial \rho}{\partial t} \quad (B.39)$$

It is, therefore, \( J' \) which satisfies the continuity equation in place of \( J \).

A modification to the method using potentials which preserves the noise properties involves correction \( \rho \) rather than \( J \). This yields an algorithm which is the same as a code from Boris [1971], except for small differences in the particle/field grids and weighting.

Langdon and Lasinski [1976] give equations for their code, “ZOHAR”, which uses the electric and magnetic fields directly, keeping in mind the noise considerations mentioned in Langdon [1972]. They use a grid in which the charge density, \( \rho \), is calculated on the particle-grid (with whole number indices in both the \( x \) and \( y \) directions); \( E_x \) and \( J_x \) (and \( B_z \), in a 2\( \frac{1}{2} \)-dimensional case) are at half steps along the \( x \) grid, \( E_y \) and \( J_y \) (and \( B_y \)) are at half steps along the \( y \) grid, and \( B_z \) (and \( E_z \), \( J_z \)) are at half steps in both directions. This allows for differenced forms of Maxwell’s equations which are second order accurate in both space in time:

\[
\frac{(B_{x,i+\frac{1}{2},j+\frac{1}{2}}^{n+\frac{1}{2}} - B_{x,i+\frac{1}{2},j+\frac{1}{2}}^{n-\frac{1}{2}})}{\Delta t} = -c(\partial_x E_y - \partial_y E_x)_{i+\frac{1}{2},j+\frac{1}{2}}^{n} \quad (B.40)
\]

\[
\frac{(E_{x,i+\frac{1}{2},j}^{n+1} - E_{x,i+\frac{1}{2},j}^{n})}{\Delta t} = (c\partial_y B_z - J_z)_{i+\frac{1}{2},j}^{n+\frac{1}{2}} \quad (B.41)
\]

\[
\frac{(E_{y,i+\frac{1}{2},j+\frac{1}{2}}^{n+1} - E_{y,i+\frac{1}{2},j+\frac{1}{2}}^{n})}{\Delta t} = (-c\partial_x B_z - J_y)_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} \quad (B.42)
\]
With $\mathbf{E}$ calculated at whole time steps and $\mathbf{B}$ calculated at half time steps. Regarding the remainder of Maxwell's equations, they show that if the divergences are correct initially, they will be correct throughout the run. The particle mover follows from Buneman [1967].

In Lembege and Dawson [1987], a one-dimensional simulation is used, with both species treated as particles. The equations are fully electromagnetic and relativistic - that is, the full set of Maxwell's equations are solved. Techniques from Lin et al. [1974] and Langdon and Lasinski [1976] are used to deal with finite-sized particles. A magnetic piston is used to generate a shock. They show non-resistive heating due to reflected ions as a main source of dissipation, with anomalous resistive effects excluded.

Unlike 1-D hybrid simulations, 1-D full particle simulations such as Lembege and Dawson [1987], and the earlier study of Biskamp and Welter [1972], show a self-reformation of the shock front. The shock causes some portion of the ion distribution to reflect, initially forming a foot region in front of the shock, but as more ions are reflected the amplitude increases to become comparable to the original shock front. This new shock front then reflects more incoming ions, causing the process to repeat.

The two-dimensional full particle code of Forslund et al. [1984] does not show this self-reformation, but Lembege and Savoini [1992] find that, rather than being an artifact of the 1-D simulations, self-reformation of the shock can occur under certain conditions in 2-D simulations as well. The authors present a two-dimensional simulation based on the previous models. Here, resistive effects can be included or excluded (in contrast to the 1-D model, where they are entirely absent) by changing the alignment of the magnetostatic field. Unlike the hybrid code of, for example, Winske and Leroy [1983], the implicit full-particle code does not include an ad-hoc resistive term. Instead, resistivity can be included self-consistently as a result of cross-field instabilities - or excluded, depending on the direction of the ambient field. (Forslund et al. [1984] compare different orientations of $\mathbf{B}$ to show the effect of cross-field instabilities on electron and ion heating.) Several studies have investigated the conditions necessary for self-reformation to appear in a simulation; the results of these studies as they relate to ion trajectories after reflection are discussed further in Section 2.3.6.
Appendix C

Derivation of Upstream Gyroradius

One of the invariants found in Section 3.2.2 is the upstream gyroradius, $\rho_u$. We now derive the form of $\rho_u$ used.

Similarly to Section 2.2, we split the ion velocity upstream of the shock into a constant guiding centre component and a gyration component:

$$v = v_{gc} + v_g$$

$$\Rightarrow v_g = v - v_\parallel - v_d \quad (C.1)$$

With the magnetic field constrained to the $xz$-plane, the parallel velocity is:

$$v_\parallel = \frac{(v \cdot B_u)B_u}{|B_u|^2}$$

$$= \frac{(\hat{x}B_x + \hat{z}B_{uz})(B_x\hat{x} + B_{uz}\hat{z})}{|B_u|^2} \quad (C.2)$$

The motional electric field is:

$$E = -V_u \times B_u$$

$$= V_u B_{uz}\hat{y} \quad (C.3)$$
Then, the drift velocity is:

\[ \mathbf{v}_d = \frac{\mathbf{E} \times \mathbf{B}}{|\mathbf{B}_u|^2} = \frac{V_u B_{uz}(B_{uz}\hat{x} - B_z\hat{z})}{|\mathbf{B}_u|^2} \]  

(C.4)

Substituting, we find:

\[
\mathbf{v}_g = \left( \hat{x} - \frac{B_z(\hat{x} B_z + \hat{z} B_{uz}) - V_u B^2_{uz}}{|\mathbf{B}_u|^2} \right) \hat{x} + \hat{y} \hat{y} \\
\quad + \left( \hat{z} - \frac{B_{uz}(\hat{x} B_z + \hat{z} B_{uz}) + V_u B_x B_{uz}}{|\mathbf{B}_u|^2} \right) \hat{z}
\]

\[
= \frac{\hat{x} B^2_{uz} - V_u B^2_{uz} - \hat{z} B_z B_{uz} \hat{x} + \hat{y} \hat{y} + \frac{\hat{z} B^2_z - \hat{x} B_z B_{uz} + V_u B_x B_{uz}}{|\mathbf{B}_u|^2} \hat{z}}{|\mathbf{B}_u|^2}
\]

\[
= \frac{B_{uz}(B_{uz}(\hat{x} - V_u) - B_z \hat{z})}{|\mathbf{B}_u|^2} \hat{x} + \hat{y} \hat{y} + \frac{B_x (B_z \hat{z} - B_{uz}(\hat{x} - V_u))}{|\mathbf{B}_u|^2} \hat{z} \]  

(C.5)

The gyroradius is:

\[ \rho_u = \frac{|\mathbf{v}_g|}{\Omega} \]  

(C.6)

where \( \Omega = \frac{q|\mathbf{B}_u|}{m} = \frac{|\mathbf{B}_u|}{m} \). Then:

\[ \rho^2_u = \frac{n^2 (B_{uz}(\hat{x} - V_u) - B_z \hat{z})^2 + |\mathbf{B}_u|^2 \hat{y}^2}{|\mathbf{B}_u|^4} \]

\[
= \frac{(B_{uz}(p_1 - n V_u) - B_z p_2) (B_{uz}(p_1 - n V_u) - B_z p_2) + |\mathbf{B}_u|^2 (p_2 + B_z z - B_{uz}^2)^2}{|\mathbf{B}_u|^4} \]  

(C.7)
Appendix D

Alternate Method for Finding the Invariants

Starting again with (3.27), (3.28), (3.32), and (3.33), differentiating the first two equations and substituting gives:

\[
\frac{d^2 x}{dp_2^2} = \frac{B_{uz}(p_2 + B_x z - B_u x)}{(\hat{m}V_u B_{uz})^2} \quad (D.1)
\]

\[
\frac{d^2 z}{dp_2^2} = \frac{-B_x (p_2 + B_x z - B_u x)}{(\hat{m}V_u B_{uz})^2} \quad (D.2)
\]

We can rearrange the first of these equations to get \(z\) in terms of \(x\) and its second derivative.

\[
z = \frac{(\hat{m}V_u B_{uz})^2}{B_x B_{uz}} \frac{d^2 x}{dp_2^2} + \frac{B_{uz}}{B_x} x - \frac{p_2}{B_x} \quad (D.3)
\]

Now we can obtain two equations for \(\frac{d^2 z}{dp_2^4}\) in terms of \(x\) and its derivatives; the first by differentiating (D.3), and the second by substituting (D.3) into (D.2).

\[
\frac{d^2 z}{dp_2^2} = \frac{(\hat{m}V_u B_{uz})^2}{B_x B_{uz}} \frac{d^4 x}{dp_2^4} + \frac{B_{uz}}{B_x} \frac{d^2 x}{dp_2^2} \quad (D.4)
\]

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\[
\frac{d^2 z}{dp_2^2} = \frac{-B_z}{B_{uz}} \frac{d^2 x}{dp_2^2} \tag{D.5}
\]

Setting these equations equal to each other gives a fourth-order differential equation in \(x\).

\[
\frac{d^4 x}{dp_2^4} + \frac{|B_u|^2}{(\bar{m}V_u B_{uz})^2} \frac{d^2 x}{dp_2^2} = 0 \tag{D.6}
\]

The general solutions to this equation take the form:

\[
x = C_1 \cos \left( \frac{|B_u|p_2}{\bar{m}V_u B_{uz}} - C_2 \right) + C_3 p_2 + C_4 \tag{D.7}
\]

From here, we can substitute the expression for \(x\) into earlier equations to find expressions for \(z\), \(p_1\), and \(p_3\) in terms of \(p_2\) and the constants of integration, and then solve for the invariants in terms of the phase variables as in the first method.
Appendix E

Solving for the Invariants
Through the Shock

The decoupling method used in Section 3.2.1 might also be applied through the shock. However, $B_z$, $\alpha$, $\phi$, and $\phi'$ are now functions of $x$, so we must modify the matrices appropriately. We start with:

$$\hat{m}V_u B_{uz} \frac{dp}{dp_2} = Kp + r(x)$$  (E.1)

where:

$$K = \begin{bmatrix}
0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 \\
0 & B_z(x)B_x & B_z(x) & 0 & 0 \\
0 & -B_z^2 & B_z & 0 & 0
\end{bmatrix}$$  (E.2)

and

$$r(x) = \begin{bmatrix}
0 \\
0 \\
\hat{m}V_u B_{uz} \\
-B_z(x)\alpha(x) - \hat{m}\phi' + B_z(x)p_2(0) \\
B_z\alpha(x) - B_zp_2(0)
\end{bmatrix}$$  (E.3)
are functions of \( x \). The eigenvalues of \( K \) are now \( \lambda = 0, 0, 0, iB_z, -iB_z \) and we have \( K = MDM^{-1} \) where:

\[
D = \begin{bmatrix}
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & iB_z & 0 \\
0 & 0 & 0 & 0 & -iB_z
\end{bmatrix}
\]  \( \text{(E.4)} \)

\[
M = \begin{bmatrix}
1 & 0 & 0 & B_z(x) & B_z(x) \\
0 & 0 & 1 & -B_z & -B_z \\
0 & 0 & -B_z & 0 & 0 \\
0 & 1 & 0 & iB_z(x)B_z & -iB_z(x)B_z \\
0 & 0 & 0 & -iB_z^2 & iB_z^2
\end{bmatrix}
\]  \( \text{(E.5)} \)

\[
M^{-1} = \frac{1}{2B_z} \begin{bmatrix}
2B_z & 2B_z(x) & \frac{2B_z(x)}{B_z} & 0 & 0 \\
0 & 0 & 0 & 2B_z & 2B_z(x) \\
0 & 0 & -2 & 0 & 0 \\
0 & -1 & -\frac{1}{B_z} & 0 & \frac{i}{B_z} \\
0 & -1 & -\frac{1}{B_z} & 0 & -\frac{i}{B_z}
\end{bmatrix}
\]  \( \text{(E.6)} \)

Now with \( q = M^{-1} p \) we have:

\[
\dot{m}V_u B_z \frac{dq}{dp_2} = Dq + s
\]  \( \text{(E.7)} \)

where:

\[
Dq = \begin{bmatrix}
q_2 \\
0 \\
0 \\
iB_z q_4 \\
-iB_z q_5
\end{bmatrix}
\]  \( \text{(E.8)} \)
\[ s = M^{-1} r(x) \]

\[
= \begin{bmatrix}
\frac{\tilde{m} V_o B_{z2} B_z(x)}{B_x^2} \\
-\tilde{m} \phi' \\
\frac{\tilde{m} V_o B_{z2}}{B_x} \\
-\tilde{m} V_o B_{z2} + i B_z \alpha(x) - i B_z p_2(0) \\
\frac{2 B_x^2}{B_x} \\
-\tilde{m} V_o B_{z2} - i B_z \alpha(x) + i B_z p_2(0) \\
\frac{2 B_x^2}{B_x}
\end{bmatrix}
\]  

(E.9)

At this point, the solution to the differential equations is analytically intractable. Some progress could perhaps be made by assuming a particular functional form for the fields; however, this is beyond the scope of the present study.
Bibliography


