Instability-enhanced friction in the presheath of two-ion-species plasmas

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Received 9 October 2014
Accepted for publication 25 November 2014
Published 20 January 2015

Abstract
The speed at which ions enter a sheath is a fundamental property of a plasma that also provides a useful boundary condition in modeling. A recent theory proposed that this can be significantly influenced by an instability-enhanced friction force arising from two-stream instabilities in the presheath when multiple ion species are present. Although experiments appeared to confirm this theory, recent particle simulations have brought it into question. We reconcile this controversy using direct numerical solutions of the dispersion relation, which show that there is a dependence on the electron–ion temperature ratio that was not considered previously. In addition, particle-in-cell simulations are used to show that ion–ion two-stream instabilities can arise near the sheath edge and generate an enhanced ion–ion friction force. Only by accounting for the instability-enhanced friction force can theory predict the simulated ion speeds at the sheath edge.

Keywords: two-stream instability, sheath, Bohm criterion

1. Introduction

Knowing the speed at which ions leave a sheath is a fundamental property of a plasma that also provides a useful boundary condition for modeling. A recent theory proposed that this can be significantly influenced by an instability-enhanced friction force arising from two-stream instabilities in the presheath when multiple ion species are present. Although experiments appeared to confirm this theory, recent particle simulations have brought it into question. We reconcile this controversy using direct numerical solutions of the dispersion relation, which show that there is a dependence on the electron–ion temperature ratio that was not considered previously. In addition, particle-in-cell simulations are used to show that ion–ion two-stream instabilities can arise near the sheath edge and generate an enhanced ion–ion friction force. Only by accounting for the instability-enhanced friction force can theory predict the simulated ion speeds at the sheath edge.

Keywords: two-stream instability, sheath, Bohm criterion

(Some figures may appear in colour only in the online journal)
drag causes only slight deviations from this prediction in weakly collisional plasmas [9]. In the other limit, complete coupling between the two ion species, such that \( V_1 = V_2 \) in equation (1), predicts flow at a common system sound speed \( c_s = \left( \frac{n_1}{n_e} c_{s1}^2 + \frac{n_2}{n_e} c_{s2}^2 \right)^{1/2} \). Although there was apparent theoretical consensus on the individual sound speed solution [1, 24], experiments in Ar\(^+\)–Xe\(^+\) plasmas measured values closer to the system sound speed [10–15]. This merging of ion speeds suggests that ion–ion friction may be playing a role in the experiments, but standard Coulomb collisions are far too weak to explain the measurements [16, 17].

A recent theory proposed that ion–ion two-stream instabilities in the presheath can cause an instability-enhanced friction (IEF) force through wave–particle scattering [16, 17]. This theory is consistent with the experimentally observed flow coupling, and experimental evidence for ion–ion two-stream instabilities using probes has also been presented [11, 18, 19]. Although experiments appeared to provide verification [18, 19], recent particle-in-cell/Monte Carlo collision (PIC-MCC) simulations by Gudmundsson and Lieberman (GL) were shown to disagree with it [20]. These simulations found no evidence of the instabilities, or enhanced friction force, which challenged the theory and raised the question of why it agrees with the experiments but not the simulations. PIC-MCC is a widely used simulation technique providing one of the most detailed descriptions of plasma kinetics, so resolving this discrepancy is a critical issue.

Here, we reconcile this apparent discrepancy. First, using exact numerical solutions of the linear dispersion relation, we show that there is a critical temperature ratio required for instability \( T_e/T_i \gg (T_e/T_i)_c \) that was not considered previously. We show that while the temperature ratio from the GL simulation [20] falls below this threshold, the exact theory still predicts instability for the parameters of the LHS experiment [14]. Second, and more importantly, we conduct new PIC-MCC simulations that confirm the presence of ion–ion two-stream instabilities near the sheath edge. We find that the ion–ion friction force is enhanced in this same region. Furthermore, the simulated ion speeds agree well with the values predicted by the IEF theory.

Two-stream instabilities arise when the differential ion flow speed exceeds a threshold condition: \( V_1 - V_2 > \Delta V_c \). Differential ion flow arises as the presheath electric field accelerates the lighter species to a faster speed (e.g., within the ballistic presheath model \( V_i = c_s \) at the sheath edge). The IEF force is predicted to prevent the differential flow from significantly exceeding the threshold condition \( V_1 - V_2 \approx \Delta V_c \). However, if \( \Delta V_c > |c_{s1} - c_{s2}| \) ions reach the sheath edge without exciting instabilities, so the traditional individual sound speed solution is expected to hold. Thus, the condition

\[
\Delta V \equiv V_1 - V_2 = \min(\Delta V_c, |c_{s1} - c_{s2}|) \quad (2)
\]

has been proposed as a second constraint that along with equation (1) provides both \( V_1 \) and \( V_2 \). Two analytic approximations have been provided for \( \Delta V_c \) based on the

\[
\frac{\Delta V_c}{T_1} = \frac{k^2}{\omega^2_{ce}} \left[ \frac{1}{2} \frac{T_e}{T_i} \frac{n_1}{n_e} Z'(\xi_1) - \frac{1}{2} \frac{T_e}{T_i} \frac{n_2}{n_e} Z'(\xi_2) \right] \quad (3)
\]

where \( \xi_1 = \frac{\Delta V (\Omega - 1/2)/\nuT_1}{\nuT_2} \), \( \xi_2 = \frac{\Delta V (\Omega + 1/2)/\nuT_2}{\nuT_1} \). \( Z'(\xi) = dZ/d\xi \) and \( Z \) is the plasma dispersion function. The parameter \( \Omega \) has been defined by the substitution

\[
\omega = \frac{1}{2} k \cdot (V_1 + V_2) + k \cdot \Delta V \Omega \quad (4)
\]

where \( \omega \) is the complex angular wave frequency. This substitution highlights the fact that the growth rate depends on \( \Delta V \) and that the most unstable wavenumber is parallel to \( \Delta V \). The assumptions leading to equation (3) are that ions have Maxwellian distribution functions, unity charge, frequencies of interest satisfy \( \omega/k\nuT_e \ll 1 \), and that the gradient scale length of plasma parameters (densities, temperatures and flow speeds) are much longer than the wavelengths of interest. The latter holds because the Debye-scale waves of interest are much shorter than the presheath. Ion–neutral collisions are neglected. We also assume that the two ion species have the same temperature \( T_1 = T_2 = T_i \).

Solutions of the dispersion relation, \( \hat{\epsilon}(\omega, k) = 0 \), computed from equation (3) are shown in figure 1 for Ar–Xe plasma and in figure 2 for He–Xe plasma, each at typical parameters for low temperature plasma experiments

\[\text{We adopt the convention that species 1 is less massive than species 2, so } V_1 > V_2.\]

\[\text{7 In our simulations we find that the He}^+ \text{ and Xe}^+ \text{ temperatures are typically within 10\% of each other.}\]
Figure 1. (a) The parameters $\Omega_1$ and $\Omega_2$ in a Ar–Xe plasma using four values of the electron temperature $T_e = 1, 0.7, 0.5$ and 0.34 eV. The differential flow was taken to be $\Delta V = c_s^1 - c_s^2 = 692, 579, 490$ and 404 m s$^{-1}$ at each electron temperature. The other parameters used were $T_i = 0.023$ eV and $n_1/n_e = 0.5$. (b) Growth rates and real frequency corresponding to the solutions from (a). (c) Magnitude of the arguments of the $Z$-functions in equation (3). (parameters given in the figure captions). One salient feature of the solutions is that the Ar–Xe growth rate becomes a purely damped solution below a modest electron temperature of approximately 0.5 eV. This indicates that there is a temperature ratio threshold that was not considered in [17]. It appears to be a possible cause of the discrepancy between the GL simulations [20] and LHS experiments [14] (this point analyzed in more detail in section 2.3).

Another important aspect is shown in panel (c) in each figure. This gives the argument of each of the $Z$-functions in equation (3). Fluid treatments of the two-stream instability arise from a large argument expansion. The figures show that the arguments are not large in the Ar–Xe case, implying that a kinetic treatment is required. The arguments are large in the He–Xe case, justifying a fluid expansion, except when the electron temperature drops too low. Reference [17] discusses the kinetic versus fluid aspect at length, where it is suggested that the magnitude of these arguments depends on the mass ratio of ion species. For disparate masses $\sqrt{M_2/M_1} \gtrsim 4$ (or $\sqrt{M_2/M_1} \lesssim 1/4$) it was suggested that the normal fluid expansion should be accurate, providing an analytic approximation for $\Delta V_c$. For similar masses $1/4 \lesssim \sqrt{M_2/M_1} \lesssim 4$ it was suggested that a different (order unity argument) expansion of the $Z$-functions was required, which led to a different analytic approximation for $\Delta V_c$. The numerical analysis shown in figures 1 and 2 largely affirms this expectation. However, the previous approximations also assumed $T_e/T_i$ to be asymptotically large. The numerical analysis shows that kinetic effects onset when the temperature ratio drops below approximately 10. This implies that there is a temperature ratio threshold for instability, and that calculating this requires a kinetic treatment. This is discussed in section 2.3.

2.2. Instability threshold: $\Delta V_c$

The instability threshold in differential flow $\Delta V_c$ provides the input to the IEF theory consisting of equations (1) and (2). This
Figure 3. (a) Critical flow difference for Ar\textsuperscript{+}–Xe\textsuperscript{+} (red) and He\textsuperscript{+}–Xe\textsuperscript{+} (blue) mixtures as a function of concentration. Dashed lines correspond to solving equation (5) with \(T_e/T_i = 7, 10, 20\) and 100, while the solid curves drop the third term in equation (5). (b) Critical flow difference for different ion mass ratios computed for large \(T_e/T_i\), obtained by dropping the third term in equation (5).

Solutions of \(\Delta V_c\) computed from equation (5) are shown in figure 3 as a function of concentration. Panel (a) shows solutions for the Ar\textsuperscript{+}–Xe\textsuperscript{+} and He\textsuperscript{+}–Xe\textsuperscript{+} mass ratios at several values of the temperature ratio. These are the mixtures that have been studied experimentally [10–14, 18, 19]. The previous approximate theories were based on the limit of asymptotically large \(T_e/T_i\), removing the third term in equation (5) [17]. Figure 3 shows that this is accurate only when the temperature ratio is sufficiently large. Panel (b) shows solutions obtained in this large temperature ratio limit (by dropping the third term in equation (5)) at several different mass ratios. The normalized critical flow difference is lower at larger mass ratios.

The temperature ratio dependence can be further quantified by identifying a critical value required for instability in the presheath. Taking the differential flow speed to be the maximum possible value at the sheath edge, \(\Delta V = |c_{s1} - c_{s2}|\), equation (5) can be solved for the critical temperature ratio \((T_e/T_i)_c\) required for the IEF effect to arise in the presheath (if \(\Delta V_c > |c_{s1} - c_{s2}|\) the entire presheath is stable). Making this substitution, the arguments of the \(Z\)-functions in equation (5) depend only on \((T_e/T_i)_c\) and \(M_1/M_2\). Figure 4 overlays the \(\Delta V = |c_{s1} - c_{s2}|\) curve on the critical flow difference plots for Ar–Xe. The intersection of these curves represent the critical temperature ratio points \((T_e/T_i)_c\).

Figure 5 shows solutions for this critical temperature ratio as a function of concentration at several ion mass ratios. For
He+–Xe+ mixtures. do not. Blue squares show the parameters of our new simulations of experiments fall in the unstable parameter space, but the simulations routine to model particle–neutral collisions [27]. No explicit This electrostatic code simulated one spatial dimension, three
domain was 10 cm with grounded absorbing walls; secondary
Coulomb collision routine was included. The simulation
is limited by the instability threshold. These were carried
out using the PHOENIX1D code previously described in [26].

Next, we present new PIC-MCC simulations to: (1) Search
for the presence of two-stream instabilities in a regime where linear theory predicts that they should be present, (2) compare
the ion–ion friction force in cases with and without instability,
and (3) test the theoretical prediction that the differential flow
speed of each ion species is expected to be determined from the
solution of $V_1 - V_2 = \Delta V_c$ and equation (1). This figure shows
that the LHS experiment [14] falls in the unstable region of this
phase-space, while the GL simulation [20] falls in the stable
region. Thus, the reported discrepancy [20] can be explained
by the assumption of an asymptotically large temperature ratio
in the previous analytic approximations [17], which misses
the temperature ratio threshold. The numerical solution of the
instability bounds shows that the IEF theory is consistent with
both the previous experiments and simulations.

3. PIC–MCC simulations

3.1. Code description

Figure 6 shows an example of simulation results where ion–ion
two-stream instabilities were observed in the presheath. The
Fourier transform of electron density fluctuations in two
domains is shown: the entrance to the presheath (4–5 cm),
where no instabilities were observed, and near the sheath edge
(0.3–1.3 cm), where a clear signature of ion–ion two-stream
instabilities was observed. These enhanced fluctuations can
be identified as ion–ion two-stream instabilities by comparing
with the frequency predicted by the linear theory. Overlaid
on this plot are the real frequency ($\omega_R$) and growth rate ($\gamma$)
predicted by a numerical solution of the linear dispersion
relation from equation (3). These were calculated using
characteristic temperatures from the center of the simulation
domain $T_e = 4.3$ eV, $T_i = 0.3$ eV, and the concentration and
flow speeds from the simulation at 0.3, 1.3 and 4 cm. No two-
stream mode exists at 5 cm because the ion flow is zero there.
The observed fluctuation spectrum near the sheath edge
agrees quite closely with the frequencies predicted by linear
theory. Some frequency broadening is predicted from linear
theory alone since the differential flow speed changes through
the domain sampled by the FFT (this is the region between the
two $\omega_R$ curves in the figure). However, some of the
frequency broadening may also be an indicator of nonlinear
effects. The range of unstable wavenumbers observed extends
beyond that predicted by the linear theory (by approximately
a factor of 2). One possible explanation is that this

3.2. Identification of two-stream instabilities

temperature ratios below the lines, the presheath is predicted to
be stable and each ion species is expected to reach its individual
sound speed at the sheath edge. For temperature ratios above
the lines, the presheath is predicted to be unstable and the speed of each ion species is expected to be determined from the
solution of $V_1 - V_2 = \Delta V_c$ and equation (1). This figure shows
that the LHS experiment [14] falls in the unstable region of this
phase-space, while the GL simulation [20] falls in the stable
region. Thus, the reported discrepancy [20] can be explained
by the assumption of an asymptotically large temperature ratio
in the previous analytic approximations [17], which misses
the temperature ratio threshold. The numerical solution of the
instability bounds shows that the IEF theory is consistent with
both the previous experiments and simulations.
Figure 6. Fourier transform of electron density fluctuations near the sheath edge (region 1) and near the bulk (region 2) in a He⁺–Xe⁺ plasma. The middle panel shows the potential normalized by the central plasma potential (19.7 V) and the flow speed profiles. Regions 1 and 2 are indicated by the gray boxes. Normalizations use the indicated sound speeds based on the simulated electron temperature of $T_e = 4.3$ eV and central (5 cm) He⁺ concentration of $n_1/n_e = 0.072$.

Figure 7. Magnitude of each term in the He⁺ momentum balance equation: Electric field force density ($-n_1q_1E$), friction force density ($R_1$) and kinetic force density ($-\int d^3v m_1v^2f_1$). (a) At concentration $n_1/n_e = 0.072$, which was a concentration at which two-stream instabilities were observed (see figure 6). The maximum linear growth rate calculated from equation (3) is also shown for this concentration. (b) At concentration $n_1/n_e = 0.9$, which was a concentration at which two-stream instabilities were not observed.

3.3. Identification of instability-enhanced friction

The ion flow speed profiles in figure 6 show that He⁺ ions are approximately 50% slower than their individual sound speed at the sheath edge, in accordance with the theoretical prediction at this concentration; see figure 8. Figure 7 shows the profile of the magnitude of each term in the time-averaged He⁺ momentum balance equation (the momentum moment of the kinetic equation):

$$\frac{d}{dx} \left( \int d^3v m_1v^2f_1 \right) - n_1q_1E = R_1.$$  \hspace{1cm} (6)

Here the friction force is the drag felt by ions, which would otherwise respond ballistically to the electric field force. It results from collisions $R_1 = \int d^3v m_1v_C C_1$, where $C_1$ is the helium collision operator, and may include contributions from wave–particle collisions when instabilities are present [35]. We do not calculate $R_1$ directly in the simulations, but rather infer this from the residual of the terms on the left side of equation (6). The 1D version is considered because the simulations have one spatial dimension.
Figure 8. He\(^+\) (red) and Xe\(^+\) (blue) ion flow speeds at the sheath edge. Data points are from PIC-MCC simulations, and solid lines are theoretical predictions of the IEF theory using two limiting values for the electron–ion temperature ratio: \(T_e/T_i = 8\) and \(15\). The system sound speed \(c_s\) is also shown (dashed line) and the speeds are normalized to \(c_s\).

The terms on the left are the force densities associated with the kinetic energy of particles and electric field, respectively. These were calculated directly from the simulation data. The data shown were averaged over 200 rf periods for a total of \(4 \times 10^6\) timesteps, and smoothed over 7 grid cells (0.7 mm). Panel (a) shows data for a 7% He\(^+\) concentration \((n_1/n_e = 0.072\)), which is the same simulation shown in figure 6 where two-stream instabilities were observed near the sheath. The friction term is the dominant force balancing the electric field near the sheath edge at this concentration. The profile of the maximum linear growth rate calculated from equation (3) using the midpoint concentration and temperatures along with the profile of \(\Delta V\) from the simulated ion speeds is also shown. Here, the friction term is strongly correlated with the instability growth rate, in accordance with the prediction of IEF. Since no explicit collision routine was included for Coulomb collisions, and since ion–neutral collision were turned off, all of the observed ion friction must arise from instability-driven fluctuations of the electric field. Panel (b) shows data for a 90% He\(^+\) concentration \((n_1/n_e = 0.9\)), which is a situation where instabilities were not observed. Here, we see that the electric field and kinetic terms directly balance, and the friction force density is negligible. This is further evidence that the friction force observed in the simulations is directly associated with the presence of the observed instabilities.

3.4. Ion flow speeds at the sheath edge

Figure 8 shows the ion flow speeds observed in multiple simulations at different ion concentrations. This provides a clear demonstration of the merging of ion speeds predicted by the IEF mechanism. Xenon ions are close to their individual sound speed for these parameters, but the helium ions clearly do not agree with either of the simple solutions that have previously been proposed, which are individual sound speeds [9] or the system sound speed [14]. The shaded regions show solutions of the IEF theory using numerical solutions of \(\Delta V\) from equation (5) and temperature ratios \((T_e/T_i)\) ranging from 8 to 15, which corresponds to the range of temperature ratios observed in the simulations for this data set. The variation in temperature ratio with concentration is caused in part by variations in the electron temperature that can be understood from particle-balance arguments [1], but also in part by variations in the ion temperature. Over this range of values, the IEF theory agrees well with the simulation data, providing the first quantitative test of the theory using PIC-MCC simulations in a situation where the two-stream instabilities arise. The error bars on the simulation points are determined from uncertainty in the sheath edge location (vertical), which we define as the location where \(n_i - n_e\) first goes to zero, and uncertainty in the concentration ratio (horizontal). The largest uncertainties in the theoretical analysis include the neglect of ion temperature corrections to the Bohm criterion in equation (1), which are of order \(T_i/T_e\) [6], and from the assumption of Maxwellian ion velocity distribution functions.

4. Summary

In conclusion, we have found the first evidence in PIC-MCC simulations for two-stream instabilities and an associated IEF force in the presheath of plasmas with two ion species. Using numerical calculations for the instability thresholds we reconciled a previously reported discrepancy between simulations and analytic approximations of the IEF theory. This disagreement arose from an assumption of large electron-to-ion temperature ratio in the approximations, but all previous simulations and experiments agree with the instability bounds of the numerical calculation. We also tested these predictions against several new PIC-MCC simulations under a variety of conditions and found good agreement with the theory.
Acknowledgments

This research was supported in part by the University of Iowa and an appointment to the US DOE Fusion Energy Postdoctoral Research Program administered by ORISE (S.D.B.). KG was supported in part by DOE grant ER55093. TL would like to thank Dr Jean-Paul Booth for access to computational resources.

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