The Role of Plasma Instabilities in Sheath Physics

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Overview

• Brief review of sheath fundamentals
• Ion sheaths: single ion species
  • Ion-acoustic instabilities
  • Influence on IVDF
• Ion sheaths: multiple ion species
  • Ion-ion two-stream instabilities
  • Instability enhanced friction
  • Role of neutrals
• Electron sheaths
  • Ion-electron two-stream instability
  • Electron-wave scattering

Take-aways:
1) Flows can drive instabilities in the presheath of low temperature plasmas at low pressure
2) Instabilities enhance particle scattering, which influences observable macroscopic fluid dynamics
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Especially the graduate students
Sheath fundamentals

Why sheaths?
Langmuir named “plasma” and “sheath”


“Except near the electrodes, where there are sheaths containing very few electrons, the ionized gas contains ions and electrons in about equal numbers, so that the resultant space charge is very small. We shall use the name plasma to describe this region containing balanced charges of ions and electrons.”

Electrons usually escape the plasma before equilibrating with ions

- Example: $T_e = 1\text{eV}, T_i = 0.03\text{eV}, \ n = 1 \times 10^{16}\text{m}^{-3}, L \approx 1\text{ m}, \text{protons}$
- Mean free paths:
  \[
  \lambda_{ee} \approx 1\text{ m} \quad \rightarrow \quad \text{Marginal e-e equilibration}
  \]
  \[
  \lambda_{ei} \approx 2000\text{ m} \quad \rightarrow \quad \text{No e-i equilibration}
  \]
  \[
  \lambda_{ii} \approx 0.001\text{m} \quad \rightarrow \quad \text{Good i-i equilibration}
  \]

- Ions equilibrate with the neutrals
  - Similar to ion-ion mean free path
  - Details depend on pressure
Plasmas are surrounded by sheaths

- **Sheath**: A narrow region of strong electric field that acts to balance electron and ion currents lost from a plasma
  - Electrons move much faster than ions
    \[
    \frac{v_{Te}}{v_{Ti}} = \frac{m_i T_e}{m_e T_i} \approx 250 \text{ (uses } T_e = 1 \text{eV)}
    \]
  - Electrons quickly charge the boundary surface
- Sheaths are an electrostatic barrier that forms naturally as ions are attracted to the surface charge
Sheaths are thin (like a skin)

• Polarization shields electric fields in plasmas
  • Debye length: \( \lambda_{De} = \sqrt{\frac{\varepsilon_0 T_e}{en}} = 740 \sqrt{\frac{T_e (eV)}{n (cm^{-3})}} \) cm
  • Example low temperature plasma: \( T_e = 1 eV, \ n = 1 \times 10^{10} cm^{-3} \):
    \( \lambda_{De} \approx 7 \times 10^{-5} m \) (tiny!)

• More complete analysis of sheath thickness (Child-Langmuir):
  \[
  \frac{l_s}{\lambda_D} = \frac{\sqrt{2}}{3} \left( \frac{2e\Delta \phi}{T_e} \right)^{3/4}
  \]

• Plasma potential: \( \Delta \phi \)
  • Determined by balancing electron and ion currents to boundary
  • A few times \( T_e \)
Presheath is a much longer region where ions are accelerated to Mach 1

- **Bohm criterion**: Ions must flow into the sheath supersonically
  - Usually it is equal to the sonic condition
  \[ V \geq c_s = \sqrt{\frac{T_e}{m_i}} \]

Bohm, in Characteristics of Electrical Discharges in Magnetic Fields, 1949

An important boundary condition - ex: determines plasma potential
Plasma potential is determined by balancing electron and ion currents

- Ions are lost at the Bohm flux:

\[ \Gamma_i \approx 0.6en \sqrt{\frac{T_e}{m_i}} \]

  - The 0.6 is from the presheath density drop
- Electrons are lost by a thermal flux, reduced by the sheath:

\[ \Gamma_e \approx en \sqrt{\frac{T_e}{2\pi m_e}} e^{-\Delta\phi/T_e} \]

  - Setting these equal gives the plasma potential:

\[ \Delta\phi = \frac{T_e}{e} \ln \left( \sqrt{\frac{\pi m_i}{8 m_e}} \right) \approx \text{few volts} \]
Summary of sheath properties

- 2 length scales
  - Sheath $\sim \lambda_D$
  - Presheath $\sim \lambda_{in} \gg \lambda_D$

- Child-Langmuir law
  \[
  \frac{s}{\lambda_D} = 0.79 \left( \frac{e \Delta \phi}{T_e} \right)^{3/4}
  \]

- Bohm criterion
  \[
  V_i \geq c_s = \sqrt{T_e / m_i}
  \]
  - Presheath potential drop
    \[
    e \Delta \phi_{ps} \geq T_e / 2
    \]
  - Ion-neutral collisions increase the potential drop
Sheath are important in many technological applications

- Microelectronics manufacturing
  - Directed ion energy enables etching large aspect ratio trenches
  - Enable Moore’s law
- Chemistry at the surface is also important
  - Reactive ion etching
  - Reaction rates depend on ion directed energy


Figure from: http://www.appliedmaterials.com/
Sheaths also influence plasma chemistry

- Transfer of plasma-generated reactive species to materials
  - Happens through a sheath
- The sheath influences the electron energy distribution function (EEDF) in the plasma
  - The EEDF controls the rate of chemical reactions
  - Modeling the EEDF is a complex plasma-boundary interaction problem, mediated by the sheath


Godyak, PRL 65, 996 (1990)
Ion sheaths: single ion species

Can flows generated near plasma boundaries excite instabilities?
If so, do the instabilities have an influence on fluid dynamics?
Linear stability will be predicted using the plasma dielectric response function

- For Maxwellian distribution functions
  \[ f_{Ms} = \frac{n_s}{\pi^{3/2} v_T^3} e^{-(v-v_s)^2/v_T^2} \]

- The plasma dielectric is
  \[ \varepsilon(k, \omega) = 1 - \sum_s \frac{\omega_{ps}^2}{k^2 v_T^2} Z'(\frac{\omega - k \cdot V_s}{k v_T}) \]

**plasma dispersion function**

\[ Z(w) = 2ie^{-w^2} \int_{-iw}^{\infty} dt \ e^{-t^2} = i \sqrt{\pi} e^{-w^2} \text{erfc}(-iw) \]

prime denotes derivative

\[ Z'(w) = \frac{dZ}{dw} = -2[1 + wZ(w)] \]

plasma frequency: \( \omega_{ps} = \sqrt{\frac{q_s^2 n_s}{\epsilon_0 m_s}} \)

thermal speed: \( v_{Ts} = \sqrt{\frac{2k_B T_s}{m_s}} \)
Ion-acoustic instabilities can arise when ions flow relative to electrons

- Low-frequency electrostatic wave: $\omega = \omega_r + i\gamma$
  - Expand for $\omega \ll k\nu_{Te}$ and $\omega \gg k\nu_{Ti}$
- Dispersion relation: $\omega_r = k \cdot V_i - \frac{k c_s}{\sqrt{1 + k^2 \lambda_{De}^2}}$
- Unstable if flow speed and temperature ratio are large enough

$$\gamma = -\frac{k c_s \sqrt{\pi/8}}{(1 + k^2 \lambda_{De}^2)^2} \left\{ \left( \frac{T_e}{T_i} \right)^{3/2} \exp \left( -\frac{T_e/T_i}{2(1 + k^2 \lambda_{De}^2)} \right) + \sqrt{\frac{m_e}{m_i}} \left( 1 - \frac{V_i}{c_s} \sqrt{1 + k^2 \lambda_{De}^2} \right) \right\}.$$
Ion-acoustic instability can be excited in presheaths

- The high temperature ratio common in low temperature plasmas makes the plasma more susceptible to instability.

Contours show lines of constant $\log_{10}(k_{\max} \lambda_{De})$.

Contours show the maximum growth rate $\log_{10}(\gamma_{\max} / \omega_{pi})$.

Baalrud, PSST 25, 025008 (2016)
Instabilities enhance Coulomb collisions

- Particle interactions are mediated by the collective motion of the intervening plasma
  - In a stable plasma, this is mostly Debye shielding
  - In an unstable plasma, particle motion excites waves that grow in amplitude as they propagate
- Leads to wave-particle collisions
  - Electrostatic waves are excited by motion of discrete particles
  - Other particles are pushed by (scatter from) these waves
  - The waves extend the effective interaction range of particles
- Wave growth eventually stops
  - Propagate out of plasma
  - Nonlinearly saturate

Baalrud, Hegna, Callen, POP 17, 055704 (2010)
Ion-acoustic instabilities may thermalize the ion distribution near the sheath edge

- Standard theory (Tonks-Langmuir) predicts that ionization and charge exchange cause the IVDF to become non-Maxwellian in the presheath
  - Ions are "born" at different points on the potential hill

- Enhanced ion-ion collisions in the presence of IA instabilities may thermalize the distribution

- 3 regions are predicted:
  a) Thermal with slow ion flow
  b) Nonthermal due to collisions
  c) Thermal again due IE collisions

Baalrud, Hegna, PSST 20, 025013 (2011)
Measurements of the IVDF appear to agree with this prediction

- Ion-neutral collisions will damp the instability
- Predicted threshold condition for neutral pressure:
  \[ p_n \geq \frac{k_B T_e}{\sigma v T_e} \sqrt{\frac{m_i n_e e^2}{\epsilon_0 m_e}}. \]

3 regions appear to be observed

Threshold trend qualitatively agrees with prediction

**Figure 3.** ivdfs of Xe ions in a \( P = 0.25 \) mTorr, \( T_e = 1.7 \) eV, \( n_e = 3.5 \times 10^9 \) cm\(^{-3}\) xenon plasma at varying distances from the sheath edge.

Different lines pertain to a proposed measure of the “degree of thermalization”
Ion-acoustic fluctuations were recently measured in the presheath

- Can’t use probes: The probe itself would excite instability!
- Laser induced fluorescence (LIF)
  - \( n_0 \sim 9 \times 10^8 \text{cm}^{-3} \quad T_e \sim 5 \text{ eV} \)
- Far from electrode
  - \( Z_{Ei} \sim 6 \text{ cm}, \lambda_{De} \sim 0.06 \text{ cm} \)

Required LIF measurements at MHz frequency!
Ion sheaths: multiple ion species

Can one ion species flowing relative to another excite instability? Does this influence the collisional coupling of the two ion species?
Many plasmas have multiple ion species

• Consider a plasma with 2 ion species
  • Ex: Ar⁺-Xe⁺ or He⁺-Xe⁺

• The Bohm criterion does not determine the speed of each species (even if equality is assumed, as expected)

\[
\frac{n_1}{n_e} \frac{c_{s1}^2}{V_1^2} + \frac{n_2}{n_e} \frac{c_{s2}^2}{V_2^2} \leq 1 \quad \text{where} \quad c_{si} = \sqrt{\frac{T_e}{M_i}}
\]

(1) If ion-ion drag is negligible, both species gain the same energy in the presheath: \( M_1 V_1^2 / 2 = M_2 V_2^2 / 2 \)

Individual sound speed solution: \( V_i = c_{si} \)

(2) If ion-ion drag is very strong: \( V_1 = V_2 \)

System sound speed solution: \( c_s = \sqrt{(n_1/n_e)c_{s1}^2 + (n_2/n_e)c_{s2}^2} \)
Is the ion-ion friction weak or strong?

• Consider typical low temperature plasma parameters:
  • Example: $T_e = 1 eV$, $T_i = 0.03 eV$, $n = 1 \times 10^{16} m^{-3}$

• Plasma kinetic theory for Coulomb collisions predicts
  • Ion-ion collision mean free path is a few cm
  • Similar to the ion-neutral collision mean free path
  • Approximately the length of the entire presheath!

• Conclusion: **Ion-ion friction is weak**
  • So it is the individual sound speed solution…right?
    $$V_1 = c_{s1} = \sqrt{\frac{T_e}{M_1}} \quad \text{and} \quad V_2 = c_{s2} = \sqrt{\frac{T_e}{M_2}}$$

Well….Let’s test it
Surprise: Measurements do not agree with individual sound speed prediction

- Argon-Xenon plasma
- Near equal ion mix (50-50)
- Ion velocities measured using laser-induced fluorescence (LIF)

Result:
- $\text{Ar}^+$ (the light species) is slowed down
- $\text{Xe}^+$ (the heavy species) is sped up

Could the ion-ion drag actually be larger than expected?

Lee, Hershkowitz, Severn APL 91, 041505 (2007)
Is ion flow stable in the presheath?

- As each ion species falls down the presheath potential, the ion flows separate
  \[ V_i \approx \sqrt{2e\Delta\phi / M_i} \]
  - Lighter species moves faster
  - Heavier species moves slower
- May excite an ion-ion two-stream instability

\[ \hat{\xi} = 1 + \frac{1}{k^2 \lambda_{De}^2} \left[ 1 - \frac{T_e}{2 T_1 n_e} Z'(\xi_1) - \frac{T_e}{2 T_2 n_e} Z'(\xi_2) \right] \]

\[ \xi_1 = \hat{k} \cdot \Delta V (\Omega - 1/2) / v_{T_1} \]
\[ \xi_2 = \hat{k} \cdot \Delta V (\Omega + 1/2) / v_{T_2} \]
\[ \omega = \frac{1}{2} k \cdot (V_1 + V_2) + k \cdot \Delta V \Omega \]
Instability is predicted in the presheath if the conditions are right

- Flow difference has to exceed a minimum value
  \[ V_1 - V_2 > \Delta V_c \]
- Species concentration can not be too dilute
- Electron-to-ion temperature ratio has to be large enough
  \[ \frac{T_e}{T_i} \geq \left( \frac{T_e}{T_i} \right)_c \]
- Instability in presheath if
  \[ \Delta V_c > |c_{s1} - c_{s2}| \]
Instabilities have been measured

- He\(^+\)-Xe\(^+\) plasma
- Observations of ~MHz range instabilities when the ion concentration of each species was similar
- A critical observation, but was not immediately connected to the ion speeds

Hershkowitz POP 12, 055502 (2007)
Instability-enhanced friction grows quickly if instabilities are present

- **Experimental parameters**
  - 50-50, Ar⁺-Xe⁺ mixture
  - Chose $\Delta V = c_{s1} - c_{s2}$

- **Stable plasma contribution is small**
  - Black solid line

- **Instability-enhanced contribution quickly becomes much larger**
  - 10s of Debye lengths of wave growth
  - Much shorter distance than the presheath length (by 100s—1000s)

Baalrud, Hegna, Callen, PRL 103, 205002 (2009)
Instability-enhanced friction limits the difference ion flow speeds

- Condition 1: Bohm criterion

\[ \frac{n_1}{n_e} \frac{c_{s1}^2}{V_1^2} + \frac{n_2}{n_e} \frac{c_{s2}^2}{V_2^2} \leq 1 \]

- Condition 2: Maximum difference of flow speeds

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

- Uniquely predicts each flow speed

- Usually need to compute \( \Delta V_c \) from kinetic theory

Baalrud, Hegna POP 18, 023505 (2011)
Results agree with experiments

- Predicts a significant influence on the ion species concentration
- Tested experimentally
  - Ar$^+$-Xe$^+$ mixture
  - Laser-induced fluorescence
  - Argon speed (circles)
  - Xenon speed (squares)
- Agrees with IE collision prediction
  - System sound speed (black)
  - Individual sound speeds (red and blue dash-dotted lines)
  - IE prediction (red and blue solid lines)

Yip, Hershkowitz, Severn PRL 104, 225003 (2010)
Particle-in-cell simulations have also been used to test the theory

- Predicted wave dispersion has been confirmed

- Predicted friction force has been confirmed

unstable conditions $n_1/n_e = 0.072$

stable conditions $n_1/n_e = 0.9$
Simulated ion speeds agree with the kinetic theory predictions

Baalrud, Lafleur, Fox and Germanchewski PSST 24, 015034 (2015)
Ion-neutral collisions can prevent the ion-ion two-stream instability

Kim, Song, Roh, Jang, Ryu, Huh and Kim, PSST 26, 06LT01 (2017)
Finite neutral pressure causes different regimes of ion flow speeds

- Theory curves modeled the instability threshold conditions including a BGK collision operator.
Our PIC simulations suggest that neutral pressure causes 4 regions

No charge exchange

with charge exchange

- The Bohm criterion itself is modified at high pressure
- Simulations agree with Godyak’s theory

\[ u_{Si} = \sqrt{\frac{1}{1 + \frac{\pi \lambda_{De}}{2 \lambda_{i-n}}}} \frac{c_{Si}}{} \]

[Godyak, Sternberg PRA 42, 2299 (1990)]

Adrian, Baalrud and Lafleur, POP 24, 123505 (2017)
PIC simulations are able to directly test the predicted IE friction force

\[
\frac{d}{dx} \left( \int d^3v \, mv^2 f_1 \right) - n_1 q_1 E = R_{1-2} + R_{1-n},
\]

Momentum balance:

(a) 0.02 mTorr
(b) 20 mTorr
(c) 55 mTorr

(d) 0.02 mTorr
(e) 20 mTorr
(f) 55 mTorr
IE Friction also acts in 3 ion species plasmas: but it’s complicated

- LIF measurements of Ar$^+$ and Xe$^+$ in an Ar-Xe-Kr mixture
  - Ar$^+$ and Xe$^+$ concentrations are equal: add Kr
- Any combination of 2 species has potential for instability
  - First assumed “passive” species is not influenced by IE friction
  - Assumption: Kr$^+$ had it’s own sound speed (no measurement)

Yip, Hershkowitz, Severn and Baalrud, POP 23, 050703 (2016)
A more detailed model constrains the speed of each species

- Assume ballistic motion applies in presheath until the threshold condition for instability is met between any 2 species
  - After instability, flow difference between each species is "locked"

\[ \Delta v_{12} = \Delta v_{13} \frac{1 - \sqrt{m_1/m_2}}{1 - \sqrt{m_1/m_3}} \]

- LIF measurements of Ar\(^+\) and Xe\(^+\) in a Ne-Ar-Xe mixture
Electron sheaths

Do electrons and ions flow relative to one another near electron sheaths?
If so, does it influence electron or ion scattering?
Electron sheaths can form near positively biased electrodes

- Potential rises from plasma to electrode
- Reflects ions, collects electrons
- Similar in many ways to an “inverted” ion sheath
  - Child Langmuir law
  - Bohm criterion $V_e \geq v_{eB}$
    $$v_{eB} = \sqrt{k_B(T_e + T_i)/m_e} \approx \sqrt{k_B T_e/m_e}$$
- However, no presheath was expected
  - Electron-electron collisions are extremely rare
  - Effusion of electrons (not diffusion)

Hood, Baalrud, Merlino, Skiff, POP 27, 053509 (2020)
The electron velocity distribution is nominally expected to be truncated

- Electron-electron mean free path is much larger than the sheath or presheath scale (recall ~1 m)
- All electrons moving toward sheath are lost, and none come back
- This \( \frac{1}{2} \) Maxwellian satisfies the Bohm criterion
  - So no electron presheath, right?
  - Is the electron distribution shifted, or just truncated?
Electron pressure gradients drive a fast electron flow towards the sheath

- Actually, there is an electron presheath!
- Reason is that electron pressure gradient cause electrons to flow

\[ V_e \frac{dV_e}{dy} = -\frac{e}{m_e} E - \frac{T_e}{m_e n_e} \frac{dn_e}{dy} - V_e (v_R + v_s) \]

- PIC simulations reveal that most of the electron drift is due to the shift rather than the truncation!
- Electron flow shift is very fast!
  - \( v \sim v_{Te} = \sqrt{T_e/m_e} \gg c_s = \sqrt{T_e/m_i} \)

FIG. 2. PIC simulation results showing that the EVDF can be modeled as a flowing Maxwellian in the electron sheath and presheath. The sheath edge is at \( y \approx 0.25 \) cm.
The electron flow excites ion-electron two-stream instabilities

- Experiments used LCIF measurements
- Electron presheath is very large (~5 times longer than an ion presheath)

Simulated

![Graphs showing ion and electron sheath](image)

Yee, Scheiner, Baalrud, Barnat, Hopkins, PSST 26, 025009 (2017)
LIF measurements have also directly measured these instabilities.
Instability-enhanced electron-electron collisions are expected to be the mechanism for thermalizing electrons

- Effusion occurs when gas escapes a container through a very small hole
  - Hole diameter much smaller than the collision mean free path
  - No drift or diffusion, just slow leaking

- Diffusion occurs when gas escapes a container through a larger hole
  - Hole diameter of the size of, or larger than, the collision mean free path
  - Diffusion causes a drift of gas out of the hole

- The electron sheath problem was expected to be a problem of effusion, but is observed to be a problem of diffusion
  - This requires sufficient electron-electron collisions to setup a fluid state
  - But the electron-electron mean free path is HUGE
  - Is this due to instability-enhanced electron scattering?
Summary

• Electrostatic instabilities excited by one species streaming relative to another arise near sheaths
  • Ion-acoustic
  • Ion-ion two stream
  • Electron-ion two stream
• These instabilities feedback to measurably influence plasma transport
  • Wave particle collisions cause thermalization
  • Instability-enhanced ion-ion friction

For more, see our recent review:
Baalrud, Scheiner, Yee, Hopkins and Barnat, PSST 29, 053001 (2020)
Thank you for attending!
The Tonks-Langmuir model is the seminal kinetic sheath theory

• Accounts for ions “born” at different locations in the presheath
  • Assumes the ions are born at rest
  • Makes the theory analytically tractable
  • Steady state
• Other generalizations have been made to account for finite temperature of ion source
A time-dependent Tonks—Langmuir model is unstable

- PIC ions, adiabatic electrons
- Instability frequency much lower than acoustic

Sheridan, Baalrud, PRE 96, 053201 (2017)
Instability due to direct energization from electric field

- Ion-acoustic instability cannot act because electrons are adiabatic
- Solve the linearized Vlasov equation with an electric field

\[
\hat{\epsilon}(k, \omega) = 1 + \frac{1}{k^2 \lambda_D^2} - \frac{\omega_{pi}^2 / (k^2 v_{Ti}^2)}{(1 - i \xi_i)} \left[ \frac{(\omega - ku_i) / kv_{Ti}}{\sqrt{1 - i \xi_i}} \right]
\]

- Electric field parameter

\[
\xi_i = \frac{2ekE/M}{k^2 v_{Ti}^2} = \frac{1}{k \lambda_i}
\]

- Causes poles to rotate in phase space

\[
E = 0 \quad eE/(T_e/\lambda_D) = -0.001
\]
Predicts a low frequency instability in qualitative agreement with the simulations.

Sheridan, Baalrud, PRE 96, 053201 (2017)