Excitation and propagation of negative-potential solitons in an electronegative plasma

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The excitation, propagation, and interaction of planar negative-potential solitary waves in a plasma containing positive ions, negative ions, and electrons (i.e., an electronegative plasma) are studied using a hybrid simulation with kinetic, particle ions, and Boltzmann electrons. Solitary waves are launched into the plasma when the potential on an initially unbiased electrode is stepped downward. They then propagate self-consistently through the ambient plasma. Results are shown for excitation and propagation as well as for overtaking collisions. During overtaking collisions, the solitons preserve their shape and speed, though they are not necessarily described by the Korteweg–deVries theory. These solitons may provide a useful diagnostic of the negative ion concentration in electronegative plasmas. © 1999 American Institute of Physics. [S0021-8979(99)01019-1]

I. INTRODUCTION

Solitary waves (SWs) in plasma are a subject of continuing interest because they lie at the intersection of plasma physics and nonlinear dynamics.1,2 (We use the term “solitary wave” to refer to any pulse-like wave of permanent profile, as well as to the special case of solitons.) In particular, negative-potential ion-acoustic SWs are easily excited in plasmas containing positive ions, negative ions, and electrons (i.e., an electronegative plasma) and have consequently been the subject of numerous experimental, analytical, and computational studies.

Experimentally,3–8 small-amplitude SWs in an electronegative plasma have been found to have properties consistent with those predicted by the Korteweg–deVries (KdV) equation or modified KdV equation. Overtaking collisions and oblique collisions between solitons have been investigated.9 In the overtaking collision, a phase shift was noted as the larger (faster) and smaller (slower) SWs exchanged positions. In two dimensions, results for launching and propagation from inner and outer corners and for planar electrodes with cylindrical perturbations10 have also been reported. In the main, the motivation for these articles was to verify the KdV theory. Consequently, it was necessary to estimate the negative ion concentration independently of the measured SW properties. However, if we accept that the theory describing SWs in an electronegative plasma is essentially correct, then the measured soliton properties can be used to infer plasma parameters, particularly the negative ion concentration.

Analytically,9–13 when the SW represents a small perturbation to the ambient plasma, the KdV equation or the modified KdV equation might apply. The properties of solutions to these equations are well known.1 When the perturbations to the plasma are large, or for certain parameter regimes in an electronegative plasma,14 the KdV theory does not apply, and equations with stronger nonlinearities must be considered. For example, finite-amplitude SWs exist with speeds just above the ion-acoustic speed for conditions where KdV solitons do not occur.15

Computationally,14–17 “collisionless” fluid simulations14–16 of the early stages of SW excitation by pulsed electrodes have been reported for a number of geometries, including planar, and inner and outer corners. One-dimensional, hybrid simulations (particle ions and Boltzmann electrons) of SW propagation and interaction in a three-component plasma have also been reported,17 as well as two-dimensional simulations modeling both launching and propagation from planar electrodes with cylindrical perturbations.8

In this article, we demonstrate that hybrid simulations (particle ions and Boltzmann electrons) are capable of reproducing experimentally observed features of negative-potential SWs in an electronegative plasma, as well as illuminating features of non-KdV SWs. These simulations bridge the gap between the simplifications of analytic theories (e.g., the KdV theory) and the complexities of real experiments. In Sec. II, we describe our model, while in Sec. III results are presented and discussed for the excitation of one-dimensional, planar SWs and for overtaking collisions.

II. MODEL

We consider an initially uniform, charge-neutral plasma containing positive ions with mass $M_+$, charge $e$ and density $n_+$, negative ions with mass $M_-$, charge $-e$, and density $n_-$, and electrons with density $n_e$. Charge neutrality requires...
where $n_{+0}$, $n_{-0}$, and $n_{e0}$ are the positive ion, negative ion, and electron densities in the ambient plasma. We assume that the ions are cold and collisionless. The electrons are in thermal equilibrium having a temperature $T_e$, so that the electron density is

$$n_e = n_{e0} \exp \left( \frac{e \phi}{kT_e} \right).$$

Initially the plasma potential $\phi=0$. At time $t=0$, the potential on an electrode abutting the plasma (i.e., the wall) is driven from $\phi_w=0$ to a negative potential $\phi_{\max}$ with a rise time $t_r$. That is, the electrode bias is

$$\phi_w = \phi_{\max} \left[ 1 - \exp (-t/t_r) \right].$$

Subsequently, a SW of negative amplitude also introduce the ion plasma frequency

$$\omega_{pi} = \frac{c_s}{\lambda_e}.$$ 

To determine the appropriate dimensionless variables for this problem, we consider the governing equation for an isolated, negative-potential, planar solitary wave of permanent profile. Poisson’s equation in a reference frame moving with the SW is

$$\frac{d^2 \phi}{d\alpha^2} - \frac{e}{\epsilon_0} \left[ \frac{n_{+0}v_0}{\sqrt{v_0^2 + 2 e \phi/M_+}} - \frac{n_{-0}v_0}{\sqrt{v_0^2 + 2 e \phi/M_-}} \right] - (n_{+0} - n_{-0}) \exp \left( \frac{e \phi}{kT_e} \right),$$

where we have used the cold ion fluid equations of continuity and motion. Positive ions encounter a potential valley and are rarefacted, while negative ions encounter a potential hill and are compressed. (Negative-potential SWs are sometimes termed “rarefactive,” to distinguish them from positive-potential SWs in which the positive ions are compressed.) Consequently, the SW has a deficit of positive ions and an excess of negative ions. Using the dimensionless variables

$$\eta = -\frac{e \phi}{kT_e} \quad \xi = \frac{x}{\lambda_e} = \frac{\epsilon_0 k T_e}{2 e^2 n_{e0}} \left( \frac{e \phi}{kT_e} \right)^{-1/2},$$

where $\lambda_e$ is the electron Debye length, Eq. (4) becomes

$$\frac{d^2 \eta}{d\xi^2} = \left[ \frac{1 + 2 \eta \mu (1 - \epsilon)}{u_0^2 \mu + \epsilon} \right]^{-1/2} \epsilon \left( \frac{1 - 2 \eta 1 - \epsilon}{u_0^2 \mu + \epsilon} \right)^{-1/2} - (1 - \epsilon) e^{-\eta},$$

with the three parameters

$$\mu = \frac{M_+}{M_+}, \quad \epsilon = \frac{n_{-0}}{n_{+0}}, \quad u_0^2 = \frac{v_0^2}{c_s^2} = \frac{v_0^2}{kT_e} \left( \frac{1 + \epsilon \mu}{M_+} \right)^{-1}.$$

Here $\mu$ is the ion mass ratio, $\epsilon$ is the negative ion concentration, and $u_0$ is the SW speed normalized by the ion-acoustic speed $c_s$. Since our simulation results depend on time, we also introduce the ion plasma frequency

$$\omega_{pi} = \frac{c_s}{\lambda_e}.$$ 

Given values of $\mu$, $\epsilon$, and $u_0$, a dimensionless SW amplitude

$$\eta_0 = -\frac{e \phi_0}{kT_e > 0},$$

must be found such that $\eta(\pm \infty) \to 0$ to obtain a negative-potential SW solution of Eq. (6). For $u_0 > 1$, the SW amplitude is a positive root of the Sagdeev potential

$$U(\eta) = \left\{ \eta_0^2(\mu + \epsilon) \right\} \left[ 1 + \frac{2 \eta \mu (1 - \epsilon)}{u_0^2 \mu + \epsilon} \right]^{1/2}$$

$$+ \frac{\epsilon u_0^2 (\mu + \epsilon)}{1 - \epsilon} \left[ 1 - \frac{2 \eta (1 - \epsilon)}{u_0^2 \mu + \epsilon} \right]^{1/2} + (1 - \epsilon)(e^{-\eta} - 1),$$

associated with Eq. (6).

In Fig. 1, we indicate the properties of solutions to Eq. (6) in $\mu-\epsilon$ parameter space, which is separated into five regions. If $\epsilon < \epsilon_{\min}$, where $\epsilon_{\min}$ is a solution of

$$(1 + \mu)^{1/2} - 1 = \frac{\epsilon_{\min}}{\epsilon + \epsilon_{\min}} \left[ \exp \left( -\frac{1}{2} \frac{\mu + \epsilon_{\min}}{1 - \epsilon_{\min}} \right) - 1 \right],$$

then Eq. (6) does not admit negative-potential SW solutions. If $\eta_0 \ll 1$ (i.e., small-amplitude solitons) and $\epsilon > \epsilon_{KdV}$, then the SW solutions of Eq. (6) are (approximately) KdV solitons, where $\epsilon_{KdV}$ is found from

![Figure 1](https://via.placeholder.com/150)
the quantity
\[ \frac{1 - \varepsilon_{KdV}}{\mu^2} - \frac{(1 + \varepsilon_{KdV}/\mu)^2}{1 - \varepsilon_{KdV}} = 0. \] (12)

This is the condition that the cubic term in the Taylor series expansion of \( U(\eta) \) vanishes. For \( \varepsilon = \varepsilon_{KdV} \), small-amplitude solitons are described by the modified KdV equation, while the quantity
\[ \varepsilon_c = \frac{(1 + \mu)^{1/2} - 1}{\mu} \] (13)

separates regions where the SW amplitude is limited from those where it is not. That is, unlike positive-potential SWs in an electropositive plasma, there is no upper limit on the SW speed in an electronegative plasma for \( \varepsilon < \varepsilon_c \). A point not always appreciated is that negative-potential SWs exist in the region \( \varepsilon_{min} < \varepsilon < \varepsilon_{KdV} \), though they are not described by the KdV theory.\[ \text{III. RESULTS AND DISCUSSION} \]

Use of the fluid model from which Eq. (6) derives to study the excitation, propagation or interaction of SWs is problematic as ion trajectories may cross or converge (especially in two and three dimensions), leading to artificial collisionality in the “collisionless” ion fluid. For example, during the launching process negative ions expelled from the high field region near the electrode may overtake slower ions at the sheath edge. We sidestep these pitfalls (though at the expense of greater noise) by using a fluid-particle hybrid code, in which the ion Vlasov equations are solved using the particle-in-cell technique. To accurately determine the ion densities, we use equal numbers of particles for each ion species irrespective of \( \varepsilon \). After the particles have been weighted to the computational grid, the ion densities are then scaled to give the correct relative values.

Using this model, we have investigated the excitation of SWs by a planar electrode as well as overtaking collisions. We assume that the ion species are \( \text{Ar}^+ \) and \( \text{SF}_6^- \), as a number of experiments have been reported for discharges made with Ar and \( \text{SF}_6 \) gases—we sidestep the question of what ion species might actually be present in such a discharge. Hence, we take \( \mu = 3.66 \). For a \( \text{K}^+ - \text{SF}_6^- \) plasma (i.e., a \( Q \)-machine plasma with \( \text{SF}_6^- \)), \( \mu = 3.77 \), so that our results may also have some application to this case, though in a \( Q \) machine the positive ion temperature is not negligible. Consequently, \( \varepsilon_{min} = 0.145 \), \( \varepsilon_c = 0.317 \), and \( \varepsilon_{KdV} = 0.542 \). We concentrate on the cases \( \varepsilon = 0.8, 0.542 \), and 0.4, where \( \varepsilon = 0.542 \) is close to the value reported in the experiments in Ref. 8. This allows us to sample three different conditions in \( \mu - \varepsilon \) parameter space (Fig. 1)—KdV solitons, modified KdV solitons, and non-KdV SWs.

A. Excitation of solitary waves

In this section we investigate the launching of SWs from a one-dimensional, planar electrode and their subsequent propagation. Electrode biases [Eq. (3)] \( \phi_{max} \) from \(-0.5 \) to \(-16 \) \( kT_e/e \) have been used. The rise time is fast, \( t_e \omega_{pi} = 1/8 \ll 1 \), so that an ion-matrix sheath will initially be formed. A computational grid spacing of \( 1/4 \lambda_e \) was used with at least 2560 grid points. The time step was \( \Delta t \omega_{pi} = 1/32 \) and 32 ion particles were initially placed uniformly in each simulation cell. The simulation was stopped at \( t \omega_{pi} = 500 \), allowing SWs and large-amplitude acoustic waves adequate time to separate.

The launching of a planar, negative-potential SW for \( \varepsilon = 0.4 \) is shown in Fig. 2, where we plot \(-e\phi/kT_e \) as a function of time and space. A large SW with a speed of 1.30 \( c_s \) and an amplitude of \(-4.4 \) \( kT_e/e \) is excited when the electrode bias is stepped to \(-8 \) \( kT_e/e \)—the SW amplitude is (for this case) approximately half the applied potential. The SW is trailed by a large amplitude ion acoustic wave packet with a speed just below \( c_s \). Such waves can be difficult to distinguish from solitons as they disperse very slowly. For \( \varepsilon < \varepsilon_{KdV} \), as is the case in Fig. 2, the trailing edge of the wave steepens as the trough behind the leading peak deepens. The potential at the edge of the sheath adjacent to the electrode fluctuates with a frequency well below than the ion plasma frequency. These fluctuations are associated with the excitation of ion acoustic waves at the sheath edge which then propagate into the density depleted region abutting the electrode. As the SW is supersonlic, it outpaces wave-like disturbances and consequently probes the unperturbed plasma.

Physically, why are solitary waves launched from a negatively-stepped electrode? When the electrode bias is stepped downward, an ion-matrix sheath forms as electrons are rapidly expelled from the neighborhood of the electrode. Positive ions are then attracted to the electrode and negative

![Fig. 2. Space-time plot of the dimensionless plasma potential \(-e\phi/kT_e \) for a negative-amplitude, one-dimensional, planar solitary wave launched from a negatively stepped electrode at \( x = 0 \). The negative ion concentration is \( \varepsilon = 0.4 \) and the asymptotic electrode bias is \( -8 \) \( kT_e/e \). Time is normalized by \( \omega_{pi}^{-1} \) and distance by \( \lambda_e \). The potential scale has been truncated to show fine detail—the solitary wave has an amplitude of \( \approx -4.4 \) \( kT_e/e \). Contours are drawn at \(-0.1 \) and \(-0.3 \) \( kT_e/e \).](image-url)
ions repelled. As positive and negative ions separate, an electric field forms that opposes the further motion of the ions and hinders sheath expansion—to collect positive ions at the electrode, negative charge must be transported into the plasma. We may say that the system is “frustrated.” The negative-potential SW is a collective plasma response addressing this conundrum. Because the SW has an excess of negative ions and a deficit of position ions, it shifts negative ions away from the electrode, and positive ions toward it, thereby facilitating sheath expansion. In addition, the negative charge near the electrode can be reduced by lowering the electron density, which is accomplished by lowering the potential (for Boltzmann electrons). This process results in the formation of a low-potential region that expands into the plasma with a speed below the ion acoustic speed.

The relation between the observed SW amplitude and speed is plotted in Fig. 3, where we compare solutions of Eq. (10) to simulation results. For \( \epsilon < \epsilon_{KdV} \), the SW amplitude remains finite as the SW speed approaches the ion acoustic speed—there is a minimum nonzero SW amplitude in this regime. There is a large spread in the curves for speeds close to the ion acoustic speed allowing different negative ion concentrations to be easily distinguished. For large speeds and amplitudes all the curves show similar asymptotic behavior. For large speeds and amplitudes all the curves show similar asymptotic behavior. For large speeds and amplitudes all the curves show similar asymptotic behavior.

The launching efficiency, which we define as the ratio of the amplitude of the largest excited SW to the excitation potential, \( \phi_0 / \phi_{max} \), is shown in Fig. 4. Importantly, for a given \( \epsilon \) the points cluster around a single value, though there is some spread with the efficiency increasing slightly with \( \phi_{max} \). For \( \epsilon = 0.8 \) the launching efficiency is greater than unity, indicating that the excited SW is larger than the excitation signal. The dependence of the launching efficiency on \( \epsilon \) is approximately linear, with an intercept on the \( \epsilon \) axis at \( \epsilon = \epsilon_{min} \) for \( \epsilon < \epsilon_{min} \) it is not possible to excite a negative-potential SW no matter how large the applied potential. We have drawn a line in Fig. 4 indicating an empirically determined maximum launching efficiency. Since the minimum SW amplitude is nonzero for \( \epsilon < \epsilon_{KdV} \) (Fig. 3) and the launching efficiency is low, the excitation signal required to launch a SW may be quite large. Further, these results represent the minimum applied bias required to excite a SW—the pre-existing sheath around a real electrode (which we do not here consider) further reduces the launching efficiency.

B. Overtaking collisions

As shown earlier, SWs are easily excited by a negatively pulsed electrode and then propagate through the ambient plasma with constant speed and amplitude. We may rightly call these SWs “solitons” if they are preserved in a collision. The history of the plasma potential during an overtaking collision is shown in Fig. 5 for \( \epsilon = 0.4 \) in the non-KdV regime. Initially, a SW of amplitude \( -1.9 \ kT_e / e \) is launched using an electrode bias \( \phi_{max} = -4 \ kT_e / e \). At \( t \omega_{pi} \approx 33 \) the electrode bias is stepped to \( -24 \ kT_e / e \) and a second, larger SW with an amplitude of \( -4.1 \ kT_e / e \) is excited. Here the launching efficiency is significantly reduced due to the pre-existing sheath. At \( t \omega_{pi} \approx 90 \) the larger SW catches up to the smaller one and the trailing SW then wanes, while the leading waxes, until \( t \omega_{pi} \approx 130 \) the larger SW leads the smaller one. The two SWs then part ways. This
collision displays the saddle topology characteristic of the nonlinear interaction between SWs. At no time during the collision do the SWs merge into a single-humped object, as would be expected for a linear superposition. (In the KdV theory, if the two solitons were derived from a two-soliton, reflectionless potential, they will overlap during an overtaking collision. Of course, it is exceedingly unlikely that two arbitrary SWs satisfy this criterion.) A nonlinear interaction between the second soliton and an ion acoustic wave occurs at $t \alpha_0 \approx 50$, and also exhibits a phases shift. The amplitude of the sum of the soliton and wave during overlap is less than that of the unperturbed soliton, emphasizing the nonlinear nature of the interaction.

There are two points worth remarking upon for the overtaking collision in Fig. 5, though neither would be remarkable if these were KdV solitons. First, the initial SWs emerge unscathed from the collision, earning the title "soliton." Second, they are shifted in phase. Both of these features are predicted by the KdV theory and seen experimentally in three-component plasmas by G. Schmidt, who also predicted that these were KdV solitons. First, the initial SWs emerge unscathed from the collision. Of course, it is exceedingly unlikely that two arbitrary SWs satisfy this criterion.) A nonlinear interaction between the second soliton and an ion acoustic wave occurs at $t \alpha_0 \approx 50$, and also exhibits a phases shift. The amplitude of the sum of the soliton and wave during overlap is less than that of the unperturbed soliton, emphasizing the nonlinear nature of the interaction.

IV. CONCLUSIONS

The hybrid simulations (Boltzmann electrons and particle ions) presented here reproduce some of the salient experimental features of negative-potential solitary waves in an electronegative plasma. In particular, solitary waves and large amplitude ion acoustic waves are found to be excited when the potential on an initially unbiased electrode is stepped downward. Such solitary waves shift positive ions toward the electrode and negative ions away from it, allowing positive ions to be collected by the electrode and moving negative ions into the ambient plasma. In an overtaking collision, the solitary waves preserve their shape and speed while undergoing a phase shift. For the case illustrated, the KdV theory does not apply. Consequently, the phase shift mechanism is more general than the KdV theory.

These solitary waves may prove to be a useful diagnostic in electronegative plasmas, in much the same way as ion acoustic waves. In particular, linear waves are characterized by their dispersion relation, while solitons are characterized by three parameters: width, amplitude, and speed, which can be determined using Eqs. (6) and (10), or from more sophisticated models. Both waves and solitons give information about the negative ion concentration, since the ion acoustic speed does not depend on the absolute densities. However, solitary waves have the advantage that they are localized entities, and therefore their measurement will give local information about the negative ion concentration. Further, negative-potential solitary waves are efficiently excited by negatively pulsing a solid electrode, which has several advantages. First, solitary waves can be launched from the plasma boundaries without the need for an internal electrode. Second, the excited electrode is hidden from the plasma by a cathodic sheath. In contrast, it is quite difficult to excite positive-potential solitary waves using a similar method since most of the applied positive bias raises the global plasma potential rather than creating a solitary wave.

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