Reduced Electron Model with Accurate Trapping Effects for Non-Linear Ion Accoustic Waves

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Introduction / Motivation

- Simulating Ion Acoustic Waves (IAWs) with fully kinetic ion and electron dynamics is very costly: electron/ion time scale separation $\sim \omega_{pe}/\omega_{\rm IAW} \sim (m_e/m_i)^{1/2} \ll 1$.
- Electrons therefore usually approximated assuming an isothermal Boltzmann fluid response.
- Fully kinetic electron simulations may however significantly differ from corresponding ones with Boltzmann electrons:
  1. The Boltzmann model cannot account for electron kinetic trapping contributions to the nonlinear frequency shift. In fact, for $ZT_e/T_i \gtrsim 10$, the positive contribution from trapped electrons dominates over the negative one from trapped ions [Berger 2013].
  2. The two electron models lead to different non-linear evolutions of driven IAWs in presence of sideband instabilities [Riconda 2005].
- **GOAL: Derive a reduced electron model which enables time stepping IAW simulations at ion time scales while correctly accounting for electron trapping effects.**

Adiabatic electron model (1-dim)

- Non-linear IAW simulations with fully kinetic electron response show that the energy distribution $f(W)$ of electrons is very close to the so-called adiabatic distribution [Dewar 1972].

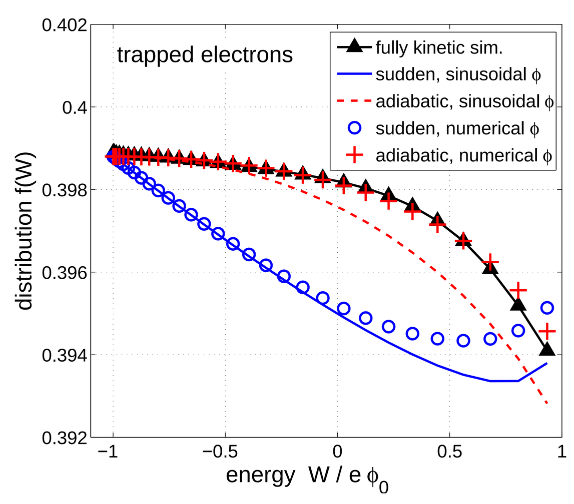


Fig. Energy distribution of trapped electrons from fully kinetic, non-linear IAW simulation using the SAPRISTI code [Berger 2013]. Similar agreement for passing particles.

- **Boltzmann** distribution:

$$f_B(W) = \frac{N_e}{(2\pi T_e/m_e)^{1/2}} \frac{\exp(-W/T_e)}{\langle \exp(e\phi/T_e)\rangle_x}$$

- **Sudden** distribution (valid if $\omega_{b,e} \ll d\log\phi_0/dt$):

$$\sum_{\sigma=\pm1} f_{\rm sud}(W,\sigma) = \frac{\left\langle \frac{\sum_\sigma f_0[v_{\rm ph}+\sigma u(x,W)]H(W+e\phi)}{u(x,W)} \right\rangle_x}{\left\langle \frac{H(W+e\phi)}{u(x,W)} \right\rangle_x},$$

- **Adiabatic** distribution (valid if $\omega_{b,e} \gg d\log\phi_0/dt$):

$$\sum_{\sigma=\pm1} f_{\rm ad}(W,\sigma) = \sum_{\sigma=\pm1} f_0(v_{\rm ph}+\sigma\bar{u})$$

u = velocity, $\sigma = {\rm sign}(u)$ and $W = m_e u^2/2 - e\phi$ = particle energy in wave frame. $\omega_{b,e}$ = bounce frequency
ϕ = electrostatic field and $v_{\rm ph}$ = (lab frame) phase velocity.
$f_0(v)$ = initial (lab frame) velocity distribution.
$\langle\cdot\rangle_x = (1/\lambda)\int_0^\lambda dx\cdot$: spatial average over one wavelength λ.

- Relation for $f_{\rm ad}$ based on the adiabatic invariance of the phase space action $\bar{u}$ (H = Heaviside):

$$\bar{u}(W) = \langle u(x,W)\,H(W+e\phi)\rangle_x = \frac{1}{\lambda}\int_0^\lambda dx\, u(x,W)\,H(W+e\phi).$$

- For IAWs one may consider limit of zero electron/ion mass ratio $\Longrightarrow v_{\rm ph}/v_{\rm th,e} \sim (m_e/m_i)^{1/2} \to 0$.
- Electron density is a non-linear functional of $\phi(x)$: $\mathcal{N}(\phi) \doteq n_e(x,t) = \int du\, f_{\rm ad}$.
- The adiabatic electron model for improved IAW simulations had already been suggested by Dewar and Valeo in 1972 [Dewar & Valeo 1973], but combined with a cold fluid ion response. A fully kinetic ion response is considered here.

Non-linear IAW simulations with kinetic ions and adiabatic electron model

Normalized system of equations for IAWs in 1-wavelength long periodic system:

Vlasov Eq. for ions: $\left[\frac{\partial}{\partial t} + v\frac{\partial}{\partial x} - \frac{\partial\phi}{\partial x}\frac{\partial}{\partial v}\right] f = 0,$

with initial Maxwellian: $f(t=0) = \sqrt{\frac{\tau}{2\pi}}\exp(-\frac{\tau v^2}{2}).$

Non-linear Poisson Eq.: $-\frac{\partial^2\phi}{\partial x^2} = \int dv\, f - \mathcal{N}(\Phi = \phi + \phi^{\rm ext}),$

with either (linear Boltzmann) $\mathcal{N}(\phi) = n_B = 1 + \phi,$

or (non-lin. Boltzmann) $\mathcal{N}(\phi) = n_B = \frac{\exp(\phi)}{(1/\lambda)\int_0^\lambda dx\exp(\phi)},$

or (Adiabatic, $f_0 = f_M$) $\mathcal{N}(\phi) = n_{\rm ad} = \sqrt{\frac{2}{\pi}}\int_{-\phi}^{+\infty}\frac{dW}{u}\exp(-\bar{u}^2/2),$

$$u = [2(W+\phi)]^{1/2}, \quad \bar{u} = \frac{1}{\lambda}\int_0^\lambda dx\, u\, H(W+\phi).$$

- **Normalizations:**
  $\hat{x} = x/\lambda_{\rm De}$, $\hat{t} = \omega_{pi}\, t$,
  $\hat{v} = v/c_s$, $\hat{u} = u/v_{\rm th,e}$,
  $\hat{W} = W/T_e$, $\hat{\phi} = e\phi/T_e$,
  $\lambda_{\rm De} = (T_e\epsilon_0/N_e e^2)^{1/2}$ = electron Debye length,
  $\omega_{pi} = [N_i(Ze)^2/m_i\epsilon_0]^{1/2}$ = ion plasma frequency,
  $c_s = (ZT_e/m_i)^{1/2}$ = ion sound speed,
  $v_{\rm th,e} = (T_e/m_e)^{1/2}$ = electron thermal velocity.
- Single effective parameter: $\tau = ZT_e/T_i$.
- **External driver** for generating propagating waves (models ponderomotive force on electrons in LPI):

$$\phi^{\rm ext}(x,t) = \phi_0^{\rm ext}(t)\cos(kx - \omega^{\rm ext} t),$$

with driver amplitude ramped up over time $\Delta t_{\rm ramp}$ and ramped down after $\Delta t_{\rm drive}$.

Properties of the adiabatic electron model

- **Conservation of mass**:

$$\langle n_{\rm ad}\rangle_x = \frac{1}{\lambda}\int_0^\lambda dx\int_{-e\phi}^{+\infty}\frac{dW}{m_e u}\sum_{\sigma=\pm1} f_0(\sigma\bar{u})$$
$$= \int_{-\infty}^{+\infty} du\, f_0(u) = {\rm const.}$$

- **Conservation of total energy**:

$$\frac{d}{dt}E_{\rm tot} = \frac{d}{dt}(P + K_i + K_e) = 0,$$

with

$$P = \frac{\epsilon_0}{2}\int_0^\lambda dx\left(\frac{\partial\phi}{\partial x}\right)^2,$$
$$K_i = \frac{m_i}{2}\int_0^\lambda dx\int_{-\infty}^{+\infty} dv\, v^2 f_i,$$
$$K_e = \frac{m_e}{2}\int_0^\lambda dx\int_{-\infty}^{+\infty} du\, u^2 f_{\rm ad}$$
$$= \frac{\lambda}{2}\int_{-e\max(\phi)}^{+\infty} dW\,\bar{u}\sum_{\sigma=\pm1} f_0(\sigma\bar{u}).$$

- **Deviation from Boltzmann model**: $|f_B - f_{\rm ad}|$ is maximum for resonant particles

$$n_{\rm ad}^{\rm res} - n_B^{\rm res} = \int_{\rm res} du\,(f_B - f_{\rm ad}) \sim (e\phi_0/T_e)^{3/2}$$

- **Non-linear kinetic frequency shift contribution from particle trapping** [Dewar 1972]:
$\delta\omega^{\rm kin} = \delta\omega_i^{\rm kin} + \delta\omega_e^{\rm kin} \sim (e\phi_0/T_e)^{1/2}$, with

$$\frac{\delta\omega_i^{\rm kin}}{kc_s} = \ominus\frac{\alpha_i}{\sqrt{2\pi}}\left(\frac{e\phi_0}{T_e}\right)^{1/2}\left(\frac{ZT_e}{T_i}\right)^{3/2}(v^2-1)e^{-v^2/2}\Big|_{\frac{c_s}{v_{\rm th,i}}}$$

$$\frac{\delta\omega_e^{\rm kin}}{kc_s} = \oplus\frac{\alpha_{\rm ad}}{\sqrt{2\pi}}\left(\frac{e\phi_0}{T_e}\right)^{1/2},$$

and $\alpha_i = \alpha_{\rm ad}$ or $\alpha_{\rm sud}$, depending on wave generation. $\alpha_{\rm ad} = 0.544$, $\alpha_{\rm sud} = 0.823$.

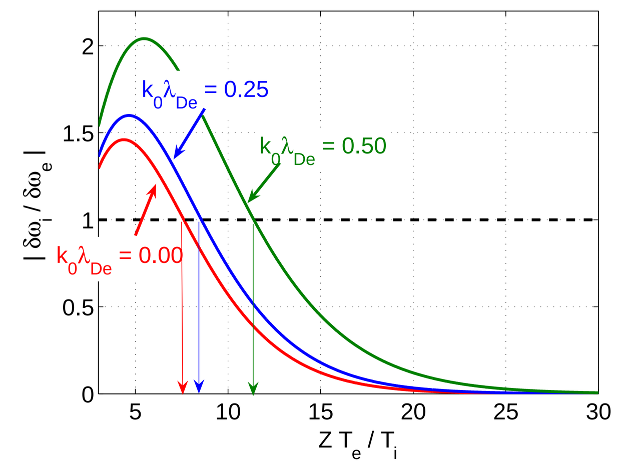


Fig. Estimated ratio of ion to electron frequency shift ([Berger 2013], assuming $\alpha_e = \alpha_i$).

Numerical approach

- **Vlasov Eq. for ions**: Semi-Lagrangian scheme based on cubic-spline interpolation with time splitting of x- and v-advection [Cheng 1976]. Time step size at ion scale: $\Delta t\,\omega_{pi} \simeq 10^{-1}$.
- **Adiabatic density** $\mathcal{N}(\phi) = n_{\rm ad}$:
  1. $\bar{u}(W) = \langle u\rangle_x$ computed for different energy levels W_l. x-integral carried out for passing orbits [$W_l > -e\min(\phi)$] with trapezoidal rule, and for trapped [$-e\max(\phi) < W_l < -e\min(\phi)$], after identify turning pts., with $\int_{x_i}^{x_{i+1}} dx\sqrt{f(x)} \simeq (2/3)(f_i + \sqrt{f_i f_{i+1}} + f_{i+1})(x_{i+1} - x_i)/(\sqrt{f_i} + \sqrt{f_{i+1}})$.
  2. Adiabatic distribution computed on grid (x_i, u_j): $f_{\rm ad}(x_i, u_j) = f_0[\bar{u}(W_{ij})]$, with $W_{ij} = u_j^2/2 - \phi(x_i)$ and $\bar{u}(W_{i,j})$ interpolated from $\bar{u}(W_l)$.
  3. $n_{\rm ad}(x) = \int du\, f_{\rm ad}(x,u)$ integrated with trapezoidal rule.
- **Non-linear Poisson Eq.** solved iteratively using Concus and Golub's scheme [Cohen 1997]:

$$(-\frac{\partial^2}{\partial x^2} + 1)\,\phi^{k+1} = n_i - \mathcal{N}(\Phi^k) + \phi^k,$$

obtained after subtracting the linearized electron response $\delta n \simeq \phi$ from both sides. $\partial^2/\partial x^2$ discretized with finite differences.

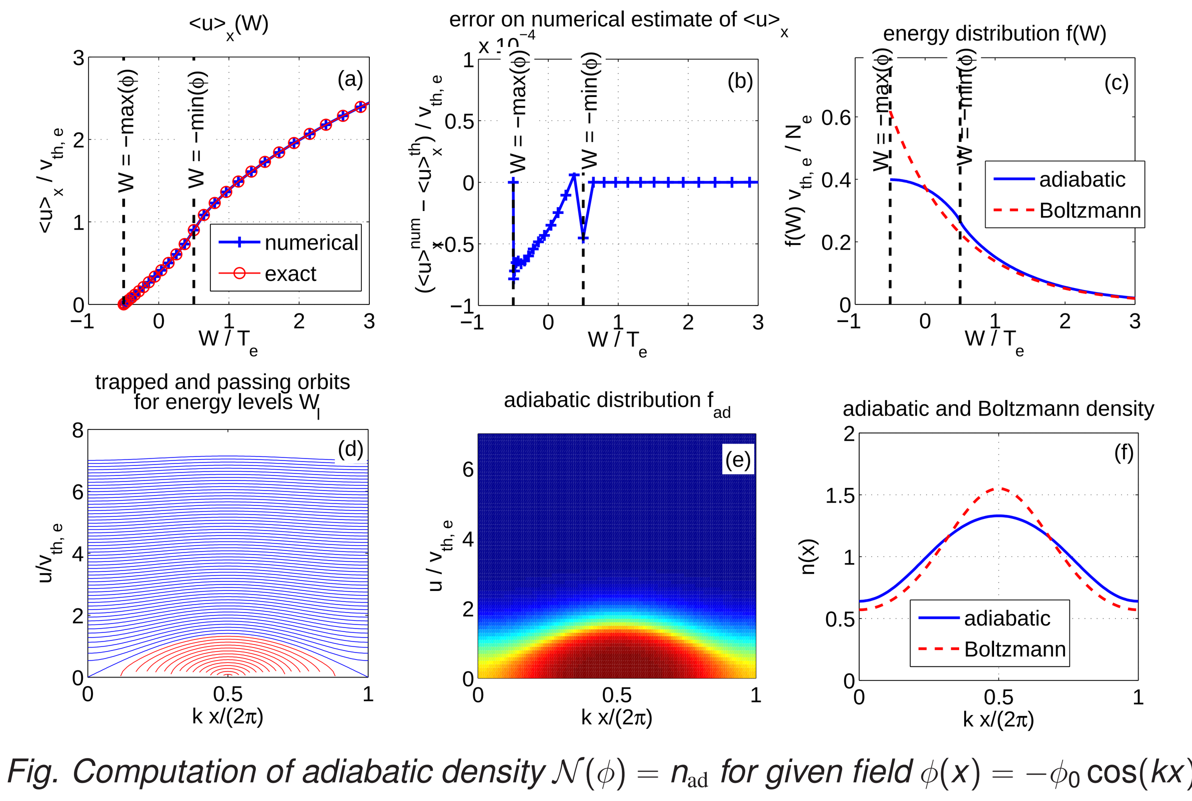


Fig. Computation of adiabatic density $\mathcal{N}(\phi) = n_{\rm ad}$ for given field $\phi(x) = -\phi_0\cos(kx)$. $e\phi_0/T_e = 0.5$, $n_x = \lambda/\Delta x = 128$, $\Delta u/v_{\rm th,e} = 0.1$, $u_{\rm max}/v_{\rm th,e} = 7$.

Analytical result for sine wave:

$\kappa^2 = 2e\phi_0/(W + e\phi_0)$,

$[F, E]$ complete elliptic int.

Passing ($0 < \kappa < 1$): $\frac{\bar{u}}{v_{\rm th,e}} = \frac{4}{\pi}\sqrt{\frac{e\phi_0}{T_e}}\frac{E(\kappa^2)}{\kappa}$

Trapped: ($\kappa > 1$) $\frac{\bar{u}}{v_{\rm th,e}} = \frac{4}{\pi}\sqrt{\frac{e\phi_0}{T_e}}\left[E(\frac{1}{\kappa^2}) + (\frac{1}{\kappa^2} - 1)F(\frac{1}{\kappa^2})\right]$

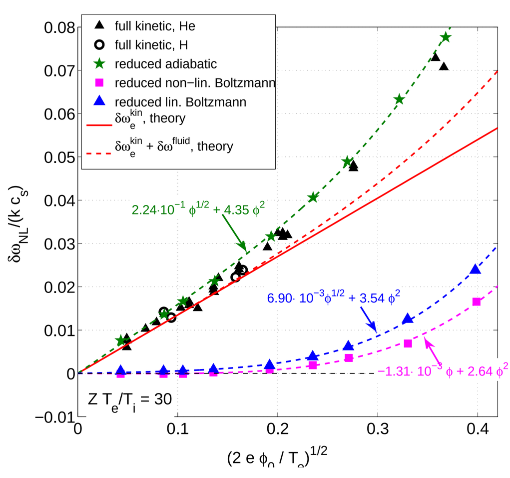
Non-linear frequency shifts of IAWs

- Waves with $k\lambda_{De} = 0.3$ driven up to different amplitudes $e\phi_0/T_e$.
- After driver is turned off, non-linear frequency $\omega_{\rm NL}(\phi_0)$ computed with Hilbert transform analysis.

Frequency shift estimate: $\delta\omega(\phi_0) = \omega_{\rm NL}(\phi_0) - \lim_{\phi_0\to0}\omega_{\rm NL}(\phi_0)$

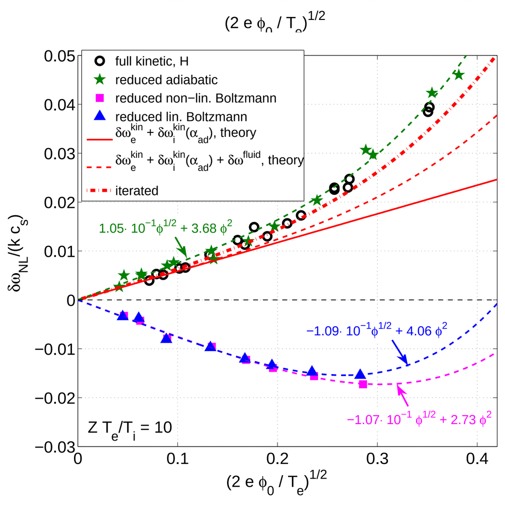
$ZT_e/T_i = 30$

- As $c_s/v_{\rm th,i} \simeq (ZT_e/T_i)^{1/2} \gg 1 \Longrightarrow \delta\omega_i^{\rm kin} \simeq 0$.
- At low amplitude, freq. shift dominated by positive electron trapping effect $\delta\omega_e^{\rm kin} \sim (e\phi_0/T_e)^{1/2}$. Absent in Boltzmann simulations.
- At high amplitude, positive contribution from $\delta\omega^{\rm fluid} \sim (e\phi_0/T_e)^2$. Theoretical estimate: $\delta\omega^{\rm fluid}/(kc_s) \simeq 1.882(e\phi_0/T_e)^2$.



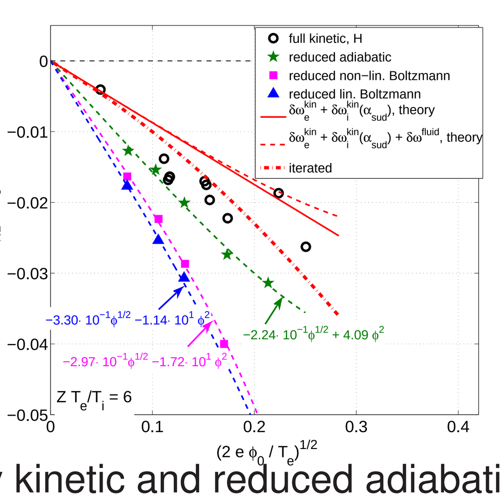
$ZT_e/T_i = 10$

- Ion and electron kinetic contributions such that $|\delta\omega_i^{\rm kin}| \sim |\delta\omega_e^{\rm kin}|$ and thus nearly compensate each other.
- Only kinetic contribution reproduced by Boltzmann simulations is negative one from ions.



$ZT_e/T_i = 6$

- $|\delta\omega_i^{\rm kin}| > |\delta\omega_e^{\rm kin}|$ and total frequency shift is negative.
- Minor differences on $\delta\omega_{\rm NL}$ between the fully kinetic and reduced electron simulations may result from non-identical driver parameters leading to an ion distribution which is more or less in the sudden or adiabatic limit $\Longrightarrow \alpha_i = \alpha_{\rm sud}$ or $\alpha_{\rm ad}$.

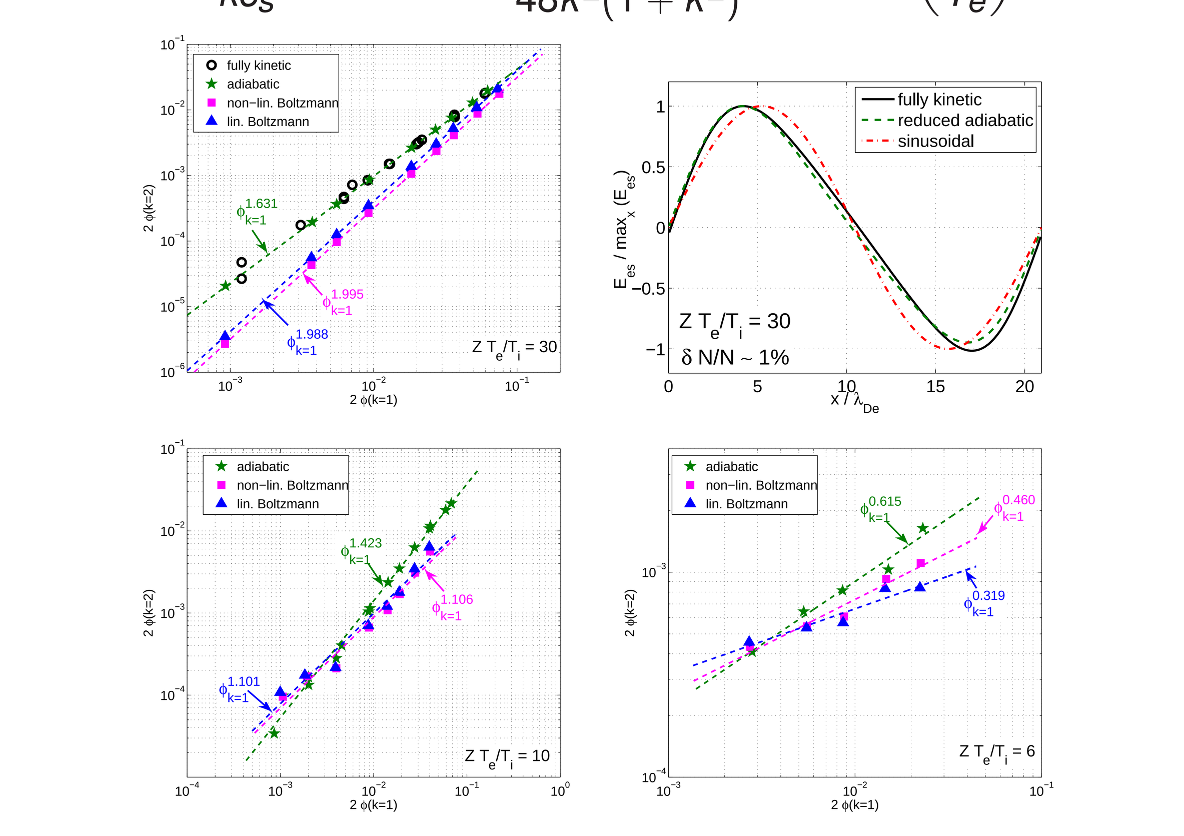


- Very good agreement between fully kinetic and reduced adiabatic simulations for all values of ZT_e/T_i.

Harmonic generation

- Non-linear fluid-like effects lead to harmonic generation: $\phi(k=2) = A_2\,\phi(k=1)^2 \Longrightarrow$ wave steepening.
- Associated contribution to frequency shift ($\tilde{k} = k\lambda_{\rm De}$):

$$\frac{\delta\tilde{\omega}^{\rm fluid}}{kc_s} = \frac{4 + 45\tilde{k}^2 + 93\tilde{k}^4 + 81\tilde{k}^6 + 24\tilde{k}^8}{48\tilde{k}^2(1+\tilde{k}^2)}\left(\frac{e\phi}{T_e}\right)^2.$$



- Only the simulations with neither electron nor ion trapping effects, *i.e.* Boltzmann runs in case $ZT_e/T_i = 30$, reproduce the scaling $\phi(k=2) \sim \phi(k=1)^2$ predicted by fluid theory.

Conclusions

- Simulations of non-linear IAWs have been carried out considering kinetic ions and a reduced electron model based on the invariance of the action $\oint u\,dx$, enabling time stepping at the ion scale.
- Excellent agreement has been shown with fully kinetic ion & electron simulations both wrt. non-linear frequency shifts (kinetic and fluid effects) as well as wrt. harmonic generation.

Outlook / Future Work

- Can the reduced adiabatic electron model be generalized in spatially 1-dim systems for handling sideband instabilities of IAWs in multi-wavelength-long systems? For carrying out simulations of Stimulated Brillouin Scattering?
- Generalization to spatially multi-dim systems?

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