Accurate representation of velocity space using truncated Hermite expansions.

Joseph Parker

Oxford Centre for Collaborative Applied Mathematics Mathematical Institute, University of Oxford

> Wolfgang Pauli Institute, Vienna 23rd March 2012



OXFORD CENTRE FOR COLLABORATIVE APPLIED MATHEMATICS

Model for ITG instabilities (from Pueschel et al., 2010)

Test problem for GENE, simplified gyrokinetic equations:

- 1D slab, (z, v_{\parallel})
- $\mathbf{B} = B\mathbf{z}$ homogeneous and static
- electrostatic: $\mathbf{E} = -\nabla \Phi$

- adiabatic electrons
- drift-kinetic ions
- quasineutral
- uniform density and temperature gradients in background
- perturbation about Maxwellian $F_0(v_{\parallel}) = \pi^{-1/2} \exp(-v_{\parallel}^2)$
- nonlinearity dropped

May also derive directly from Vlasov equation and quasineutrality.

Electrostatic limit of Belli & Hammett (2005) model

Model for ITG instabilities (from Pueschel et al., 2010)

Linearized kinetic equation

$$\frac{\partial F_1}{\partial t} + \alpha_i v_{\parallel} \frac{\partial F_1}{\partial z} + \left[\omega_n + \omega_{T_i} \left(v_{\parallel}^2 - \frac{1}{2} \right) \right] i k_y \Phi F_0 + \tau_e \alpha_i v_{\parallel} \frac{\partial \Phi}{\partial z} F_0 = 0$$

Quasineutrality

$$\Phi = \int_{-\infty}^{\infty} F_1 \, \mathrm{d} v_{\parallel}.$$

Parameters

 $\begin{array}{ll} \omega_n = 1, & \text{normalized density gradient} \\ \omega_{T_i} = 10, & \text{normalized ion temperature gradient} \\ k_y = 0.3, & \text{perpendicular wavenumber} \\ \tau_e = 1, & \text{species temperature ratio} \ (T_i = T_e) \\ \alpha_i = 0.34 & \text{nondimensional constant: velocity and length scales} \end{array}$

Wave-like solutions

$$F_{1} = f(v_{\parallel}) \exp\left(i\left(k_{\parallel}z - \omega t\right)\right)$$

Leads to eigenvalue problem,

$$L_0 f = \omega f$$

where
$$L_0 f = \alpha_i k v_{\parallel} f + \left[\omega_n + \omega_{T_i} \left(v_{\parallel}^2 - \frac{1}{2} \right) \right] k_y \Phi F_0 + \tau_e \alpha_i k v_{\parallel} \Phi F_0$$

L real \implies eigenvalues in complex conjugate pairs \implies **no damping** So actually want to solve,

$$\lim_{\epsilon \to 0} L_{\epsilon} f = \omega f, \quad \text{ for } \quad L_{\epsilon} = L_0 + i\epsilon C$$

where *C* is collisions, *e.g.* Lénard–Bernstein or BGK. Breaks symmetry, so decay rate may tend to nonzero limit as $\epsilon \to 0$.



Discretization

• Keep $\exp(ik_{\parallel}z)$ behaviour, represent v_{\parallel} on a uniform grid,

$$\Phi = \sum_{i=1}^{N} \Delta v f(v_i)$$

Obtain linear ODE system

$$\frac{\partial f}{\partial t} = i M f, \qquad M \text{ real } N \times N \text{ matrix}$$

• Matrix eigenvalue problem (quicker than running IVPs):

$$-i\omega f = \frac{\partial f}{\partial t} = iMf$$

Growth rate is $\gamma = \max \Im(\omega)$, for $\omega \in \operatorname{spectrum}(M)$.

Matrix M depends on:

- All parameters, particularly parallel wavenumber.
- **Discretization** and **resolution** of grid in v_{\parallel} .

ОССАМ 뜫



- Capture growth, but convergence slow with N.
- No decay.
 - $\epsilon \to 0$ at fixed N resolution.
 - Need to restore collisions.



Fine scales develop as $\Im(\omega) \to 0$.

ОССАМ

Hermite expansion in velocity space Use expansion in asymmetric Hermite functions,

$$f(v) = \sum_{m=0}^{\infty} a_m \phi_m(v), \quad \phi^m(v) = \frac{H_m(v)}{\sqrt{2^m m!}}, \quad \phi_m(v) = F_0(v)\phi^m(v)$$

Bi-orthogonal polynomials with Maxwellian as weight function

$$\int_{-\infty}^{\infty} \phi_m \phi^n \, \mathrm{d}v = \delta_{mn}$$

Recurrence relation

$$v\phi_m = \sqrt{\frac{m+1}{2}}\phi_{m+1} + \sqrt{\frac{m}{2}}\phi_{m-1}$$

 \implies particle streaming becomes mode coupling

Represent velocity space scales,

$$H_m(v) \propto \cos\left(v\sqrt{2m} - \frac{m\pi}{2}\right), \text{ as } m \to \infty$$

large $m \implies$ fine scales

Relative Entropy and Free Energy Relative entropy is

$$R[F|F_0] \equiv \int_{-\infty}^{\infty} F \log\left(\frac{F}{F_0}\right) - F + F_0 \, \mathrm{d}v$$
$$= \int_{-\infty}^{\infty} F \log F \, \mathrm{d}v + 2U + \text{function(density)}$$

Expansion $F = F_0 + \epsilon F_1$ gives (at leading order)

$$R[F|F_0] = \frac{\epsilon^2}{2} \int_{-\infty}^{\infty} \frac{F_1^2}{F_0} \,\mathrm{d}v = \frac{\epsilon^2}{2} \sum_{m=0}^{\infty} a_m^2 + \mathcal{O}(\epsilon^3)$$

Define free energy of each Hermite mode, E_m ,

$$E = \sum_{m=0}^{\infty} E_m,$$
 with $E_m = \frac{1}{2} |a_m|^2$

cf. energy spectra in Fourier space for Navier-Stokes turbulence.

Moment system

Replace $F_0 \equiv \phi_0$ and v with Hermite functions

$$\frac{\partial F_1}{\partial t} + i\alpha_i k v F_1 + ik_y \Phi \left[\omega_n \phi_0 + \frac{\omega_{T_i}}{\sqrt{2}} \phi_2 \right] + i \frac{k \tau_e \alpha_i \Phi}{\sqrt{2}} \phi_1 = 0$$

Put $F_1 = a_m \phi_m$ (implicit sum over repeated *m*)

$$\frac{\partial \mathbf{a_m}}{\partial t}\phi_{\mathbf{m}} + i\alpha_i k v \mathbf{a_m} \phi_{\mathbf{m}} + ik_y \Phi \left[\omega_n \phi_0 + \frac{\omega_{T_i}}{\sqrt{2}}\phi_2\right] + i\frac{k\tau_e \alpha_i \Phi}{\sqrt{2}}\phi_1 = 0$$

Use recurrence relation on particle streaming

$$\frac{\partial a_m}{\partial t}\phi_m + i\alpha_i k a_m \left(\sqrt{\frac{m+1}{2}}\phi_{m+1} + \sqrt{\frac{m}{2}}\phi_{m-1}\right) + \ldots = 0$$

Gives infinite set of coupled algebraic equations for $\{a_n\}$.

ОССАМ 👯

System of equations for expansion coefficients

$$\begin{split} \omega a_m &= \left(\sqrt{\frac{m+1}{2}} a_{m+1} + \sqrt{\frac{m}{2}} a_{m-1}\right) \\ &+ \underbrace{\frac{k_y}{\alpha_i k_{\parallel}} \left[\omega_n a_0 \delta_{m0} + \frac{\omega_{T_i} a_0}{\sqrt{2}} \delta_{m2} \right]}_{\text{driving}} + \underbrace{\frac{\tau_e a_0}{\sqrt{2}} \delta_{m1}}_{\text{Boltzmann response}} \end{split}$$

We have also used $\phi^0 \equiv 1$, so that,

$$\Phi = \int_{-\infty}^{\infty} F_1 \phi^0 \, \mathrm{d}v = \sum_{m=0}^{\infty} \int_{-\infty}^{\infty} a_m \phi_m \phi^0 \, \mathrm{d}v = a_0$$

ОССАМ

23rd March 2012 12 / 34

Matrix equation



Simple Truncation

$$\begin{pmatrix} \frac{\omega_{n}k_{y}}{\alpha_{i}k_{\parallel}} & \frac{1}{\sqrt{2}} & & \\ \frac{\tau_{e}}{\sqrt{2}} + \frac{1}{\sqrt{2}} & & 1 & \\ \frac{k_{y}\omega_{T_{i}}}{\sqrt{2}\alpha_{i}k_{\parallel}} & 1 & & \sqrt{\frac{3}{2}} & \\ & & \sqrt{\frac{3}{2}} & & \sqrt{2} \\ & & & \sqrt{2} & \end{pmatrix} \mathbf{a} = \omega \mathbf{a}$$

• Assume $a_{N+1} = 0$ at point of truncation. Last row of matrix:

$$\sqrt{\frac{N+1}{2}}a_{N+1} + \sqrt{\frac{N}{2}}a_{N-1} = \omega a_N$$

• Equivalent to discretization on Gauss–Hermite points $\{v_j\}$



• Growing mode: a_m decay as m increases $\implies a_{N+1} \approx 0$ is okay • (Not) decaying mode **not resolved**

Collisions

- Free energy should cascade to large *m* (fine scales in *v*).
- Free energy has nowhere to go when $a_{N+1} = 0$.
- Restore collisions:

$$\frac{\partial F_1}{\partial t} + \left[\omega_n + \omega_{T_i}\left(v_{\parallel}^2 - \frac{1}{2}\right)\right]ik_y\Phi F_0 + i\alpha_ikv_{\parallel}F_1 + i\tau_e\alpha_ikv_{\parallel}\Phi F_0 = C[F_1]$$

Desirable properties for $C[F_1]$

conserves mass, momentum and energy

$$\int C[F_1] \,\mathrm{d}v = \int v C[F_1] \,\mathrm{d}v = \int v^2 C[F_1] \,\mathrm{d}v = 0$$

• satisfies a linearized *H* theorem:

$$\frac{\mathrm{d}R}{\mathrm{d}t} = \epsilon^2 \int_{-\infty}^{\infty} \frac{F_1 C[F_1]}{F_0} \,\mathrm{d}v \leqslant 0$$

represents small-angle collisions (contains v-derivatives)

Lénard–Bernstein (1958) collisions

Simple member of linearized Landau/Fokker-Planck class:

$$C[F_1] = \nu \frac{\partial}{\partial v} \left[vF_1 + \frac{1}{2} \frac{\partial F_1}{\partial v} \right]$$

- collision frequency ν
- Hermite functions are eigenfunctions:

$$C\left[a_m\phi_m\right] = -\nu m a_m\phi_m$$

 \implies easy to implement in Hermite space

- Conserves mass, but not momentum or energy
- Satisfies a linearized *R* theorem:

$$\frac{\mathrm{d}R}{\mathrm{d}t} = -\epsilon^2\nu\sum_m m|a_m|^2\leqslant 0$$

ОССАМ 👯

Lénard–Bernstein in Hermite space

$$\begin{pmatrix} \frac{\omega_{n}k_{y}}{\alpha_{i}k_{\parallel}} & \frac{1}{\sqrt{2}} & & \\ \frac{\tau_{e}}{\sqrt{2}} + \frac{1}{\sqrt{2}} & -i\nu & 1 & & \\ \frac{k_{y}\omega_{T_{i}}}{\sqrt{2}\alpha_{i}k_{\parallel}} & 1 & -2i\nu & \sqrt{\frac{3}{2}} & & \\ & & \sqrt{\frac{3}{2}} & -3i\nu & \ddots & \\ & & & \ddots & & \sqrt{\frac{N}{2}} \\ & & & & \sqrt{\frac{N}{2}} & -iN\nu \end{pmatrix} \mathbf{a} = \omega \mathbf{a}$$

- matrix now complex
- roots *not* in complex-conjugate pairs \implies can find negative

growth rates

OCCAM

• (we can manually conserve momentum and energy)

Lénard-Bernstein in Hermite space

$$\begin{pmatrix} \frac{\omega_n k_y}{\alpha_i k_{\parallel}} & \frac{1}{\sqrt{2}} & & \\ \frac{\tau_e}{\sqrt{2}} + \frac{1}{\sqrt{2}} & \noti & \\ \frac{k_y \omega_{T_i}}{\sqrt{2}\alpha_i k_{\parallel}} & 1 & \cancel{2i} & \sqrt{\frac{3}{2}} & \\ & & \sqrt{\frac{3}{2}} & -3i\nu & \ddots & \\ & & & \ddots & \sqrt{\frac{N}{2}} \\ & & & & \sqrt{\frac{N}{2}} & -iN\nu \end{pmatrix} \mathbf{a} = \omega \mathbf{a}$$

- matrix now complex
- roots *not* in complex-conjugate pairs \implies can find negative

growth rates

• (we can manually conserve momentum and energy)

ОССАМ 👯



If collision frequency ν large enough to get $k_\parallel>4$ correct, then shape for $k_\parallel<4$ distorted.



- resolves dissipative scales
- expensive: 300 modes



OCCAM 👯

Hypercollisions Would prefer:

low modes undamped
 high modes strongly damped

 \ldots whatever the truncation point N

Iterate Lénard–Bernstein collisions:

$$\mathcal{L}[F_1] = \frac{\partial}{\partial v} \left(vF_1 + \frac{1}{2} \frac{\partial F_1}{\partial v} \right), \qquad C[F_1] = -\nu (-N)^{-n} \mathcal{L}^n[F_1]$$
(like *hyperdiffusion*: $-(-\nabla^2)^n$ in physical space)

Hermite functions are still eigenfunctions:

$$C\left[a_m\phi_m\right] = -\nu\left(\frac{m}{N}\right)^n a_m\phi_m$$

ν sets the decay rate of the highest mode

- linearized R-theorem: $\frac{\mathrm{d}R}{\mathrm{d}t}=-\epsilon^2\nu\sum_{m=0}^\infty\left(\frac{m}{N}\right)^n|a_m|^2\leqslant 0$
- n = 1 corresponds to Lénard–Bernstein collisions.
- two parameters: $n \approx 6$, $\nu \approx 10$ (robust to variation)

ОССАМ



- Captures decaying parts of spectrum.
- Excellent fit, fast convergence.
- Appropriate for nonlinear problems.
- Two parameters, n, ν , robust to variation.



- Low moments largely undamped
- Damping at high m, for any N.



- Low moments largely undamped
- Damping at high m, for any N.

Energy equations and theoretical spectra Equation for coefficients, valid for $m \ge 3$,

$$\omega a_m = \left(\sqrt{\frac{m+1}{2}}a_{m+1} + \sqrt{\frac{m}{2}}a_{m-1}\right) + \operatorname{driving} + \operatorname{Boltzmann} \operatorname{response}$$

Treat as a finite difference approximation in continuous m.

Energy equation for $E_m = |a_m|^2/2$ (Zocco & Schekochihin, 2011) $\frac{\partial E_m}{\partial t} + \frac{\partial}{\partial m} \left(\sqrt{2m}E_m\right) = -2\nu \left(\frac{m}{N}\right)^n E_m.$

For a mode with growth rate γ ,

$$E_m = \frac{C}{\sqrt{2m}} \exp\left(-\frac{\gamma}{|\gamma|} \left(\frac{m}{m_{\gamma}}\right)^{1/2} - \left(\frac{m}{m_c}\right)^{n+1/2}\right),$$

with the cutoffs,

$$m_{\gamma} = \frac{1}{8\gamma^2}, \qquad m_c^{(n+1/2)} = \left[\frac{N^n (n+1/2)}{\nu\sqrt{2}}\right]$$

Energy equations and theoretical spectra Equation for coefficients, valid for $m \ge 3$,

$$\omega a_m = \left(\sqrt{\frac{m+1}{2}}a_{m+1} + \sqrt{\frac{m}{2}}a_{m-1}\right) + \text{hypercollisions}$$

Treat as a finite difference approximation in continuous m.

Energy equation for $E_m = |a_m|^2/2$ (Zocco & Schekochihin, 2011) $\frac{\partial E_m}{\partial t} + \frac{\partial}{\partial m} \left(\sqrt{2m}E_m\right) = -2\nu \left(\frac{m}{N}\right)^n E_m.$

For a mode with growth rate γ ,

$$E_m = \frac{C}{\sqrt{2m}} \exp\left(-\frac{\gamma}{|\gamma|} \left(\frac{m}{m_{\gamma}}\right)^{1/2} - \left(\frac{m}{m_c}\right)^{n+1/2}\right),$$

with the cutoffs,

$$m_{\gamma} = \frac{1}{8\gamma^2}, \qquad m_c^{(n+1/2)} = \left\lfloor \frac{N^n (n+1/2)}{\nu\sqrt{2}} \right\rfloor$$





How strong should collisions be?

- We can find the collision strength required for a given resolution.
- Write hypercollisions as,

$$C[F_1] = -\nu(-\mathcal{L})^n[F_1]$$

(*i.e.* remove N^{-n} , damping strength expressed just by ν .)

Need to resolve collisional cutoff,

$$N > m_c = \left(\frac{(n+1/2)}{\nu\sqrt{2}}\right)^{1/(n+1/2)} \to \infty \text{ as } \nu \to 0$$

• Need infinite resolution to resolve collisionless case.

ОССАМ 👯

29/34



Weaker collisions \implies finer scales in spectra



- $\bullet\,$ a range of ν give the correct growth rate
- range extends to smaller ν as N increases

Hypercollisions on other grids

• Easiest to implement in Hermite space:

$$C[a_m] = -\nu (m/N)^n a_m$$
$$C[\mathbf{a}] = D\mathbf{a}$$

- But may be used on any grid.
- Map function values f to Hermite space by a = Mf, collide and map back,

$$C[\mathbf{f}] = M^{-1}DM\mathbf{f}$$

• Only need to calculate $M^{-1}DM$ once.



Example: hypercollisions implemented on a uniform grid.

ОССАМ 뜫

Summary

- 1D model for ITG instability
 - ightarrow velocity space discretization \implies eigenvalue problem
 - \succ finite composition of normal modes \implies no Landau damping
- Hermite representation
 - in decaying modes, have energy pile-up at small scales
- Damping with collisions
 - Lénard–Bernstein collisions
 - finds damping, but requires $\mathcal{O}(100)$ terms
 - hypercollisions
 - excellent agreement with dispersion relation
 - theoretical expression for eigenfunctions
 - * only ~ 10 terms
 - robust parameters
 - easy to implement in Hermite space
 - can use on any grid
- "Vanishing collisions" is different from "collisionless".

References

- BELLI, E. A. & HAMMETT, G. W. (2005) A numerical instability in an ADI algorithm for gyrokinetics. *Computer Physics Communications* **172** (2), 119–132.
- LANDAU, L. D. (1946) On the Vibrations of the Electronic Plasma. *Journal of Physics-U.S.S.R.* **10** (25).
- LÉNARD, A. & BERNSTEIN, I. B. (1958) Plasma oscillations with diffusion in velocity space. *Physical Review* **112** (5), 1456–1459.
- PUESCHEL, M. J., DANNERT, T. & JENKO, F. (2010) On the role of numerical dissipation in gyrokinetic Vlasov simulations of plasma microturbulence. *Computer Physics Communications* **181**, 1428–1437.
- VAN KAMPEN, N. G. (1955) On the Theory of Stationary Waves in Plasmas. *Physica* **21**, 949–963.
- ZOCCO, A. & SCHEKOCHIHIN, A. A. (2011) Reduced fluid-kinetic equations for low-frequency dynamics, magnetic reconnection, and electron heating in low-beta plasmas. *Physics of Plasmas* **18** (10), 102309.

Supported by Award No KUK-C1-013-04 from King Abdullah University of Science and Technology (KAUST).

ОССАМ 뜫

Drift approximation in the Vlasov equation

$$\mathbf{E}_{\perp} + \frac{\mathbf{v} \times \mathbf{B}}{c} = 0, \quad \mathbf{v} = v_{\parallel} \hat{\mathbf{z}} - \frac{c}{B^2} \nabla \Phi \times \mathbf{B}, \quad \mathbf{B} = B \hat{\mathbf{z}}, \quad \mathbf{E} = -\nabla \Phi.$$

Vlasov equation becomes

$$\frac{\partial f}{\partial t} + \left(v_{\parallel} \hat{\mathbf{z}} - \frac{c}{B^2} \nabla \Phi \times \mathbf{B} \right) \cdot \nabla f - \frac{q}{m} \frac{\partial \Phi}{\partial z} \frac{\partial f}{\partial v_{\parallel}} = 0.$$

Perturb about stationary equilibrium, $f(\mathbf{x}, \mathbf{v}, t) = F_0(\mathbf{x}, \mathbf{v}) + \epsilon F_1(\mathbf{x}, \mathbf{v}, t)$ Impose density and temperature gradients in x,

$$\frac{\partial F_0}{\partial x} = -\frac{1}{L} \left[\omega_n + \omega_{T_i} \left(\frac{v_{\parallel}^2 + v_{\perp}^2}{v_{\rm th}^2} - \frac{3}{2} \right) \right] F_0$$

Assume a Fourier mode in $y: \partial_y \mapsto ik_y$. Integrate out perpendicular directions in **v**.

$$\frac{\partial F_1}{\partial t} + \left[\omega_n + \omega_{T_i}\left(v_{\parallel}^2 - \frac{1}{2}\right)\right]ik_y\Phi F_0 + \alpha_i v_{\parallel}\frac{\partial F_1}{\partial z} + \tau_e\alpha_i v_{\parallel}\frac{\partial \Phi}{\partial z}F_0 = 0$$

Quasineutrality Poisson's equation

$$\nabla^2 \Phi = 4\pi q (n_i - n_e),$$

Boltzmann electrons

$$n_e = \bar{n}_e \exp\left(\frac{q\Phi}{T_e}\right)$$

Nondimensionalize (with $\epsilon = \rho_s/L$)

$$\frac{\epsilon T_e}{4\pi \bar{n}_i q^2 \rho_s L^2} \nabla^2 \Phi = \left(1 + \epsilon \int_{-\infty}^{\infty} F_1 \, \mathrm{d}v\right) - \frac{\bar{n}_e}{\bar{n}_i} \exp\left(\epsilon \Phi\right).$$
$$\epsilon^2 \nabla_{\perp}^2 \Phi = \left(1 - \frac{\bar{n}_e}{\bar{n}_i}\right) + \epsilon \left(\int_{-\infty}^{\infty} F_1 \, \mathrm{d}v - \frac{\bar{n}_e}{\bar{n}_i}\Phi\right) + \mathcal{O}(\epsilon^2).$$

 $\Phi,$ potential for electrostatic perturbation

$$\Phi = \int_{-\infty}^{\infty} F_1 \, \mathrm{d} v_{\parallel}.$$