The Entropy Paradox, Steady-State Statistical Balances, and Sampling Noise [a]

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Introduction

Question:

Does noise enhance or reduce diffusion?

What does noise mean?

In the context of PIC simulation, noise means extra fluctuations due to Monte Carlo sampling error. See G. Hu and J. A. Krommes, Generalized weighting scheme for δf particle-simulation method, Phys. Plasmas 1, 863 (1994).

Hu & Krommes showed that one can develop a kinetic theory of sampling noise quite analogous to the classical plasma kinetic theory of fluctuations due to particle discreteness. (The details will not be discussed here. . .)

After more than a decade, there is still confusion [and lots of (oral) noise].

Issue: Role of sampling noise in gyrokinetic particle simulation

- **Assertions:** Extra noise should
  1. increase turbulent flux;
  2. decrease turbulent flux.
- General arguments:
  - Increase — more noise $\Rightarrow$ more dissipation $\Rightarrow$ more flux (entropy argument)
  - Decrease — more noise $\Rightarrow$ more resonance broadening $\Rightarrow$ wipe out turbulent drive $\Rightarrow$ less flux

There are various paradoxes, so it's easy to get confused.

A difficulty is that saturated, turbulent, steady states are not in thermal equilibrium.

Warnings:

- Cannot (blindly) use fluctuation–dissipation theorem (FDT).
- There is no simple "thermodynamics" of a nonequilibrium steady state.

Possibilities:

- Generalize FDT $\Rightarrow$ steady-state spectral balance [entirely nontrivial, but foundations are well understood, even in the presence of discreteness/sampling effects (Rose, 1979)]
- Entropy considerations.

I will not resolve anything in this talk. My goals are to emphasize that one must be careful and that there are subtleties, but also that a systematic framework does exist for discussing these issues.

The standard entropy-balance argument is a red herring, and can be easily misinterpreted.

General form of the evolution equation for "entropy" $\mathcal{S}$ (a certain quadratic functional of the fluctuations):

$$\frac{\partial \mathcal{S}}{\partial t} = \kappa\Gamma - \mathcal{D}. \tag{1}$$

Here

$$\kappa \text{ — gradient drive (e.g., } L_n^{-1} \text{ or } L_T^{-1}) \tag{2a}$$

$$\Gamma \text{ — turbulent flux} \tag{2b}$$

$$\mathcal{D} \text{ — dissipation} \tag{2c}$$

The Entropy Paradox: If $\mathcal{D} \equiv 0$ and $\Gamma \neq 0$, then $\mathcal{S}$ increases indefinitely (incompatible with assumption of steady state). So for a steady state to exist, there must always be dissipation. (Truly collisionless simulations are suspect.) Then

$$0 = \kappa\Gamma - \mathcal{D}. \tag{3}$$

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The steady-state entropy balance is true, but its interpretations can be confusing.

$$\boxed{0 = \kappa\Gamma - \mathcal{D}.} \tag{4}$$

Interpretations:

× 1. $\mathcal{D} \Rightarrow \kappa\Gamma$ (more dissipation ⇒ more flux).

✓ 2. $\kappa\Gamma \Rightarrow \mathcal{D}$
(flux determines dissipation; no info about actual value of Γ)

See J. A. Krommes and G. Hu, The role of dissipation in simulations of homogeneous plasma turbulence, and resolution of the entropy paradox, Phys. Plasmas 1, 3211 (1994).

It's all about energy transfer:

Saturation ⇒ transfer (in $\vec{k}$ space) ⇒ dissipation.

Simple statistical models can be instructive.

Generic primitive amplitude equation:

$$\partial_t \psi - \underbrace{L\psi}_{\text{linear physics}} + \underbrace{\vec{V} \cdot \vec{\nabla} \psi}_{\text{nonlinear advection}} = 0. \tag{5}$$

The mean field evolves according to

$$\partial_t \langle \psi \rangle - L \langle \psi \rangle + \partial_x \underbrace{\langle \delta V_x \delta \psi \rangle}_{\Gamma^{(\kappa)}} = 0. \tag{6}$$

Turbulent fluctuations obey

$$\partial_t \delta\psi - L\delta\psi + \underbrace{\delta\vec{V} \cdot \vec{\nabla}\langle\psi\rangle}_{-\delta f^{(\kappa)}} + \underbrace{\vec{\nabla} \cdot (\delta\vec{V}\delta\psi) - \partial_x \Gamma}_{\Sigma^{(\mathrm{nl})}\delta\psi - \delta f^{(\mathrm{nl})}} = 0, \tag{7}$$

or

$$\partial_t \delta\psi - L\delta\psi + \underbrace{(\underbrace{\Sigma^{(\mathrm{nl})}}_{\text{“}k_\perp^2 D^{(\mathrm{nl})}\text{”}} + \underbrace{\Sigma^{(\mathrm{s})}}_{\text{“}k_\perp^2 D^{(\mathrm{s})}\text{”}})}_{\text{coherent dissipation}} \delta\psi = \underbrace{\delta f^{(\mathrm{nl})} + \delta f^{(\kappa)} + \delta f^{(\mathrm{s})}}_{\text{incoherent (internal) forcing}}. \tag{8}$$

The fluctuation-induced transport coefficients can come from either comparable scales or shorter ones.

- $D^{(\mathrm{nl})}$: $\mathsf{DW}_{\vec{p}} + \mathsf{DW}_{\vec{q}} = \mathsf{DW}_{\vec{k}}$ (large-scale turbulent diffusion)
- $D^{(\mathrm{s})}$: short-scale noise $\Rightarrow$ large-scale diffusion.

  Just like classical transport theory:

  sub-Debye-scale fluctuations $\Rightarrow$ Braginskii transport coefficients.

Turbulent steady states are described by the ***spectral balance equation.***

$$\partial_t \delta\psi - L\delta\psi + (\Sigma^{(\mathrm{nl})} + \Sigma^{(\mathrm{s})})\delta\psi = \delta f^{(\mathrm{nl})} + \delta f^{(\kappa)} + \delta f^{(\mathrm{s})}. \quad (9)$$

Now introduce

$$C(t,t') \text{ — two-time correlation function } \langle \delta\psi(t)\delta\psi(t')\rangle \quad (10a)$$

$$R(t;t') \text{ — two-time (renormalized) response function} \quad (10b)$$

and also the noise covariances $F(t,t') \doteq \langle \delta f(t)\delta f(t')\rangle$. **Then, in steady state, one has the spectral balance equation**

$$C(\omega) = \underbrace{R(\omega)}_{\text{diss.}}\underbrace{[F^{(\mathrm{nl})}(\omega) + F^{(\kappa)}(\omega) + F^{(\mathrm{s})}(\omega)]}_{\text{positive-definite forcing}}\underbrace{R^*(\omega)}_{\text{diss.}}. \quad (11)$$

More noise $\Rightarrow$ more fluctuations (and flux)? . . . No, not necessarily. (Need to know how R scales with fluctuation level.)

The spectral balance equation can be paradoxical.

Model $F^{(\kappa)}(\tau) \approx 2\kappa\Gamma^{(\kappa)}\delta(\tau)$ and $F^{(\mathrm{s})}(\tau) \approx 2\kappa\Gamma^{(\mathrm{s})}\delta(\tau)$. Assume

$$C(\tau) = [R(\tau) + R(-\tau)]I, \tag{12a}$$

$$F^{(\mathrm{nl})}(\tau) = [\Sigma^{(\mathrm{nl})}(\tau) + \Sigma^{(\mathrm{nl})}(-\tau)]I \tag{12b}$$

(the last form is necessary for energy conservation). Then

$$\underbrace{[R(\omega) + R^*(\omega)]I}_{C(\omega)} = \{\underbrace{[\Sigma^{(\mathrm{nl})}(\omega) + \Sigma^{(\mathrm{nl})*}(\omega)]I}_{F^{(\mathrm{nl})}(\omega)} + 2\kappa(\Gamma^{(\kappa)} + \Gamma^{(\mathrm{s})})\}|R|^2(\omega). \tag{13}$$

Since

$$R(\omega) = \frac{1}{-i\{\omega - iL + i[\Sigma^{(\mathrm{nl})}(\omega) + \Sigma^{(\mathrm{s})}(\omega)]\}}, \tag{14}$$

one has

$$R + R^* = \frac{2\,\mathrm{Re}(-L + \Sigma^{(\mathrm{nl})} + \Sigma^{(\mathrm{s})})}{|\omega - iL + i\Sigma^{(\mathrm{nl})} + i\Sigma^{(\mathrm{s})}|^2} = 2\,\mathrm{Re}(-L + \Sigma^{(\mathrm{nl})} + \Sigma^{(\mathrm{s})})|R|^2. \tag{15}$$

The two-time spectral balance leads to the one-time entropy balance.

Equation (13) then becomes

$$[-2\,\mathrm{Re}\,L + 2\,\mathrm{Re}(\cancel{\Sigma^{(\mathrm{nl})}} + \Sigma^{(\mathrm{s})})]|R|^2 I = 2\,\mathrm{Re}\,\cancel{\Sigma^{(\mathrm{nl})}}|R|^2 I + 2\kappa(\Gamma^{(\kappa)} + \Gamma^{(\mathrm{s})})|R|^2. \tag{16}$$

Hence

$$\underbrace{\mathrm{Re}(-L + \Sigma^{(\mathrm{s})})I}_{\text{dissipation } \mathcal{D}} = \underbrace{\kappa(\Gamma^{(\kappa)} + \Gamma^{(\mathrm{s})})}_{\kappa\Gamma}. \tag{17}$$

The two-time spectral balance is compatible with macroscopic entropy balance, but it does not determine the turbulent flux.

To actually determine the fluctuation level I or the turbulent flux $\Gamma^{(\kappa)}$, one must look at the equal-time spectral balance equation.

$$\frac{\partial I}{\partial t} - 2\gamma I + 2\,\mathrm{Re}(\Sigma^{(\mathrm{nl})} + \Sigma^{(\mathrm{s})})I = 2(F^{(\mathrm{nl})} + F^{(\mathrm{s})}) \tag{18}$$

or

$$\frac{\partial I}{\partial t} = 2\gamma I + 2\underbrace{(F^{(\mathrm{nl})} - \mathrm{Re}\,\Sigma^{(\mathrm{nl})} I)}_{\substack{-\alpha I^2 \\ -k_\perp^2 D^{(\mathrm{nl})} I}} + 2(\underbrace{F^{(\mathrm{s})}}_{q>0} - \underbrace{\mathrm{Re}\,\Sigma^{(\mathrm{s})}}_{k_\perp^2 D^{(\mathrm{s})}} I). \tag{19}$$

Kadomtsev:

- $\gamma < 0$: $I = q/|\gamma|$
- $\gamma > 0$: $I = \gamma/\alpha$.

The turbulent diffusion must be calculated self-consistently.

Let $I \sim \overline{V}^2$. Then the turbulent diffusion coefficient is

$$D^{(\mathrm{nl})} = \overline{V}^2 \tau_{\mathrm{ac}}, \quad \text{where} \quad \tau_{\mathrm{ac}} \sim \frac{1}{k_\perp^2 D^{(\mathrm{nl})} + k_\perp^2 D^{(\mathrm{s})}}. \tag{20}$$

Thus (upon solving the self-consistent equation for $D^{(\mathrm{nl})}$)

$$D^{(\mathrm{nl})} \approx \overline{V}/k_\perp - \frac{1}{2} D^{(\mathrm{s})}. \tag{21}$$

For fixed $\overline{V} \sim \sqrt{I}$, $D^{(\mathrm{nl})}$ is reduced by the sampling noise.

It's trickier to calculate the fluctuation level:

$$k_\perp^2 D^{(\mathrm{nl})}[I] = \gamma - k_\perp^2 D^{(\mathrm{s})} + F^{(\mathrm{s})}/I, \tag{22}$$

or

$$\underbrace{\overline{V}/k_\perp}_{\propto \sqrt{I}} = \gamma/k_\perp^2 - \underbrace{\left(\frac{1}{2} D^{(\mathrm{s})} - F^{(\mathrm{s})}/I k_\perp^2\right)}_{\text{sign?}}. \tag{23}$$

Note that $F^{(\mathrm{s})}$ is largely independent of I, so $F^{(\mathrm{s})}/I$ is probably small. If so, I is reduced by the presence of noise.

Now we can inquire about the turbulent flux.

$$\Gamma^{(\kappa)} = \langle \delta V_x \delta\psi \rangle \tag{24a}$$

$$= \int d\vec{x}' \, \mathcal{V}(\vec{x}, \vec{x}') \langle \delta\psi(\vec{x}', t) \delta\psi(\vec{x}, t) \rangle \tag{24b}$$

$$= \sum_{\vec{k}} \mathcal{V}_{\vec{k}} C_{\vec{k}} \tag{24c}$$

$$\propto I. \tag{24d}$$

- This is the **total** I, calculated in the presence of any sampling noise.
- In this simple generic model, if I is reduced, then $\Gamma^{(\kappa)}$ is also.
- In multifield models, one must worry about phase relations.
- There's no getting around a calculation substantially more detailed than the sketch given here.

Discussion

Observations:

- The calculation of steady-state spectra and fluxes is a difficult problem in nonequilibrium statistical dynamics.
- Steady-state spectral balances are tricky (with or without sampling noise).
- Entropy balance does not help one determine the size of the turbulent flux.
- The two-time spectral balance $C = RFR^*$ does not imply that more noise means a larger fluctuation level (or larger flux).
- The turbulent diffusion coefficient $D^{(\mathrm{nl})} = \overline{V}^2 \tau_{\mathrm{ac}}$ is nontrivial because $\tau_{\mathrm{ac}} = \tau_{\mathrm{ac}}[D^{(\mathrm{nl})}, D^{(\mathrm{s})}]$ (so if noise reduces τ_{ac}, $D^{(\mathrm{nl})}$ will also be reduced).

Conclusions (for a very simple, generic model):

- For fixed fluctuation level, $D^{(\mathrm{nl})}$ is reduced by noise.
- Probably $D^{(\mathrm{nl})}$ itself is also reduced by noise.
- That implies that the spectral level will be reduced.
- And then the turbulent flux Γ is also reduced.

References

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