

# Turbulent fluxes and entropy production rate

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## Motivation

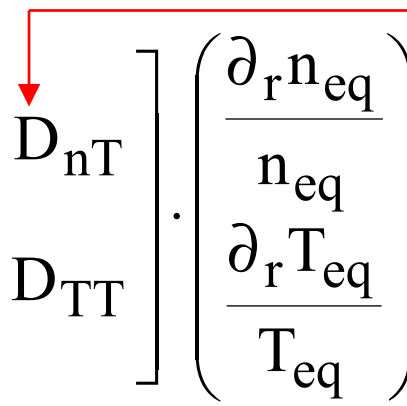
- Particle and heat fluxes versus density and temperature gradients?
- Turbulence EquiPartition Theory (fluid) Isichenko and Yankov 97

$$\Gamma = -D_{\text{turb}} \left( \partial_r n_{\text{eq}} + \frac{2}{L_{\nabla B}} n_{\text{eq}} \right)$$

$$Q = -\frac{1}{\zeta - 1} D_{\text{turb}} \left( \partial_r T_{\text{eq}} + (\zeta - 1) \frac{2}{L_{\nabla B}} T_{\text{eq}} \right) ; \quad \zeta = \frac{5}{3}$$

- Traditional formulation

$$\begin{pmatrix} \frac{\Gamma}{n_{\text{eq}}} \\ \frac{Q}{n_{\text{eq}} T_{\text{eq}}} \end{pmatrix} = - \begin{bmatrix} D_{nn} \\ D_{Tn} \end{bmatrix} \cdot \begin{pmatrix} \frac{\partial_r n_{\text{eq}}}{n_{\text{eq}}} \\ \frac{\partial_r T_{\text{eq}}}{T_{\text{eq}}} \end{pmatrix}$$



Heat pinch

Weiland & Nordman 93

Thermodiffusion

B. Coppi & Spight 78,

Tang et al. 86, Terry 89,

Waltz & Dominguez 89

Nordman, Weiland and Jarmèn 90

## Motivation (cont.)

- TEP and thermodiffusion terms are additive in particle flux Baker and Rosenbluth 00
  - Raises several questions:
    - what is the thermodynamical meaning of TEP terms?
    - does Onsager symmetry principle apply?
    - implications for the heat flux
    - are pinches consistent with the second principle?
- calculate entropy production rate.

# Outline

- Experimental evidence of off-diagonal terms in particle flux.
- Introduction to pinch mechanisms: Turbulence Equipartition Theory. Extension to interchange turbulence: curvature and thermodiffusion.
- Entropy production rate: fluid and kinetic theories.
- Examples: particle ( $e/D$ ) and impurity transport.

# Turbulence EquiPartition Theory

- ExB convection in an inhomogeneous magnetic field

Isichenko and Yankov 97, Naulin 98.

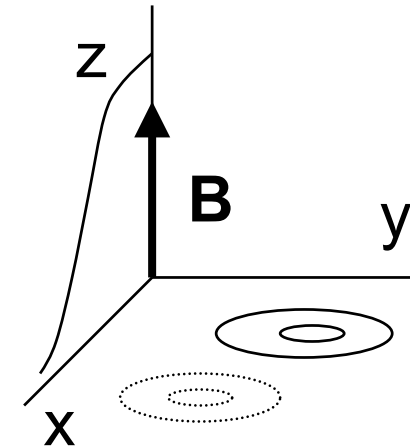
$$\partial_t n + \nabla \cdot (n \mathbf{v}_E) = 0 \quad ; \quad \mathbf{v}_E = \frac{\mathbf{B}}{B^2} \times \nabla \phi$$

- Equivalent to the advection of  $n/B$

$$(\partial_t + \mathbf{v}_E \cdot \nabla) \left( \frac{n}{B} \right) = 0$$

- Quasi-linear theory

$$\partial_t n_{eq} = \partial_x D_{turb} B \partial_x \left( \frac{n_{eq}}{B} \right)$$



- Relaxes toward canonical profile  $n_{eq} = n_{can} = B(x)$

## A step further : 2D interchange turbulence

- Equations for density and temperature Braginskii 65

$$\frac{d_t n}{n} = -\kappa \cdot \left( \nabla \phi + \frac{T}{e} \frac{\nabla n}{n} + \frac{\nabla T}{e} \right)$$

$$\frac{d_t T}{T} = -\kappa \cdot \left( (\zeta - 1) \nabla \phi + (\zeta - 1) \frac{T}{e} \frac{\nabla n}{n} + (2\zeta - 1) \frac{\nabla T}{e} \right)$$

$$d_t = \partial_t + \mathbf{v}_E \cdot \nabla \quad ; \quad \kappa = \lambda \frac{2}{B} \left( \frac{\mathbf{B}}{B} \times \frac{\nabla B}{B} \right) \quad ; \quad \zeta = \frac{5}{3}$$

- Curvature terms come from compressibility. Yancov  
 $\lambda=1/2$ , Weiland model  $\lambda=1$ , trapped electrons  
 $\lambda=1/4+2s/3$  ( $s=r dq/q dr$ ) → link between density and current See e.g. H. Weisen 04, GLF23: another function....
- Here  $\lambda$  and adiabatic index  $\zeta > 1$  are free parameters.

## Turbulent fluxes

- Expression of fluxes

$$\left( \begin{array}{c} \frac{\Gamma}{\bar{n}_{eq}} \\ \frac{Q}{\bar{n}_{eq} \bar{T}_{eq}} \end{array} \right) = - \sum_{\mathbf{k}\omega} i \frac{|\tilde{v}_{E,\mathbf{k}\omega}|^2}{D_{\mathbf{k}\omega}} \left[ \begin{array}{c} \omega - (2\zeta - 1)\omega_d \\ \omega_d \\ \frac{\omega - \omega_d}{\zeta - 1} \end{array} \right] \cdot \left( \begin{array}{c} \frac{\partial_r \bar{n}_{eq}}{\bar{n}_{eq}} \\ \frac{\partial_r \bar{T}_{eq}}{\bar{T}_{eq}} \end{array} \right)$$

$$\bar{n} = \frac{n}{n_{can}} \quad \bar{T} = \frac{T}{T_{can}}$$

$$n_{can} = n_0 \exp \left\{ - \frac{2}{R_0} \int_0^r \lambda dr \right\} \quad T_{can} \propto n_{can}^{\zeta-1}$$

- **Onsager symmetry is found.** Does not guarantee 2nd principle is respected  $\rightarrow$  entropy production rate.

## TEP limit

- When  $\omega \gg \omega_D$

$$d_t \bar{n} = 0 \quad ; \quad d_t \bar{T} = 0 \quad ; \quad d_t = \partial_t + \mathbf{v}_E \cdot \nabla$$

- Leads to turbulent diffusion equation

$$\begin{pmatrix} \Gamma \\ Q \end{pmatrix} = - \begin{bmatrix} D_{\text{turb}} & 0 \\ 0 & \frac{1}{\zeta - 1} D_{\text{turb}} \end{bmatrix} \begin{pmatrix} \partial_r \bar{n}_{\text{eq}} \\ \bar{n}_{\text{eq}} \partial_r \bar{T}_{\text{eq}} \end{pmatrix}$$

$$D_{\text{turb}} = \sum_{\mathbf{k}} \frac{|\tilde{\mathbf{v}}_{E\mathbf{k}}|^2}{\Delta\omega_{\mathbf{k}}}$$

- Diffusion applies on profiles normalised to canonical values: thermodynamical forces.



## Equivalence with pinch formulation

- Equivalent to particle curvature pinch

$$\Gamma = -D_{\text{turb}} \partial_r \bar{n}_{\text{eq}} = -D_{\text{turb}} \left( \partial_r n_{\text{eq}} + \frac{2\lambda}{R_0} n_{\text{eq}} \right)$$

- Heat pinch also predicted

$$Q = -\frac{1}{\zeta - 1} D_{\text{turb}} n_{\text{eq}} \left( \partial_r T_{\text{eq}} + \frac{2\lambda}{R_0} (\zeta - 1) T_{\text{eq}} \right)$$

- Quasi-linear theory not mandatory. Works also for fractional kinetics.

## Entropy production rate

- Total entropy  $S = \int d^3\mathbf{x} n \text{Log}(T n^{1-\zeta}) / (\zeta - 1)$

$\partial_t S = 0 \rightarrow$  does not tell much.

e.g. Hazeltine and Meiss 2003

- Entropy for profiles  $S_{\text{eq}} = \frac{1}{\zeta - 1} \int dV n_{\text{eq}} \text{Log}(T_{\text{eq}} n_{\text{eq}}^{1-\zeta})$

$$\partial_t S_{\text{eq}} = - \int dV n_{\text{eq}} \left\{ \frac{\Gamma}{\bar{n}_{\text{eq}}} \frac{\partial_r \bar{n}_{\text{eq}}}{\bar{n}_{\text{eq}}} + \frac{Q}{\bar{n}_{\text{eq}} \bar{T}_{\text{eq}}} \frac{\partial_r \bar{T}_{\text{eq}}}{\bar{T}_{\text{eq}}} \right\}$$

- $\partial_t S_{\text{eq}} > 0$  whatever the spectrum of fluctuations
- Consistent with definition of thermodynamical fluxes and forces.

## General form of fluxes

- Practical expressions of fluxes

$$\begin{pmatrix} \frac{\Gamma}{\bar{n}_{eq}} \\ \frac{Q}{\bar{n}_{eq} \bar{T}_{eq}} \end{pmatrix} = - \begin{bmatrix} D_{nn} & D_{nT} \\ D_{nT} & D_{TT} \end{bmatrix} \cdot \begin{pmatrix} \frac{\partial_r \bar{n}_{eq}}{\bar{n}_{eq}} \\ \frac{\partial_r \bar{T}_{eq}}{\bar{T}_{eq}} \end{pmatrix}$$

$$D_{nn} \approx D_{turb} \quad ; \quad D_{TT} \approx \frac{1}{\zeta - 1} D_{turb}$$

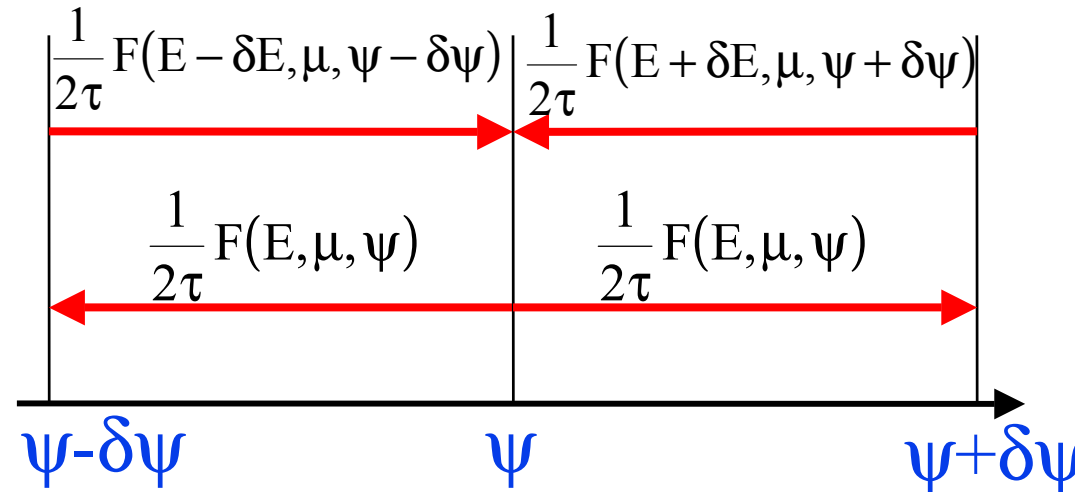
$$D_{nT} \approx \left\langle \frac{\omega}{\omega_d} - \zeta \right\rangle = \sum_{\mathbf{k}} \frac{|\tilde{v}_{E\mathbf{k}}|^2}{\Delta\omega_{\mathbf{k}}} \frac{2(\omega_{\mathbf{k}} - \zeta\omega_d)\omega_d}{\Delta\omega_{\mathbf{k}}^2}$$

- $D_{nT}$  sign depends on fluctuation spectrum. Electron pinch velocity is inward for phase velocities in the ion diamagnetic direction.

# Turbulence EquiPartition - Kinetics

Isichenko, Gruzinov & Diamond 96 - Baker & Rosenbluth 98

- Trapped particles : adiabatic invariant  $J_{//}(E, \mu, \psi) = \oint m v_{//} d\ell$
- Energy variation  $(\partial_E J_{//})\delta E + (\partial_\psi J_{//})\delta\psi = 0 \rightarrow \delta E = \Omega_d \delta\psi$



- Transport equation  $\partial_t n + \partial_\psi \Gamma = 0$

$$\Gamma = -D \int \frac{dE d\mu}{\Omega_b} (\partial_\psi F + \Omega_d \partial_E F) \quad ; \quad D = \frac{\delta\psi^2}{2\tau}$$

## General QL expression for the kinetic entropy production rate

- If a tokamak, the entropy production rate is always **positive** when using a quasi-linear kinetic theory

$$\partial_t S_{\text{eq}} = \pi \int d^3 \mathbf{J} (2\pi)^3 F_{\text{eq}} \sum_{\mathbf{n}\omega} |h_{\mathbf{n}\omega}|^2 \delta(\omega - \mathbf{n} \cdot \boldsymbol{\Omega}) [\mathbf{n} \cdot \partial_{\mathbf{J}} \text{Log}(F_{\text{eq}})]^2$$

Diagram illustrating the components of the equation:

- Action variables (points to  $\int d^3 \mathbf{J}$ )
- Hamiltonian components (points to  $F_{\text{eq}}$ )
- Resonances (points to  $\delta(\omega - \mathbf{n} \cdot \boldsymbol{\Omega})$ )
- Equilibrium distribution function (points to  $F_{\text{eq}}$ )

Samain 70

## Entropy production rate also involves canonical profiles

- Trapped particles

$$\partial_t S_{\text{eq}} = \pi \int dV n_{\text{eq}} \sum_{\mathbf{k}\omega} |v_{E,\mathbf{k}\omega}|^2 \left\langle \delta(\omega - \omega_d) \left\{ \frac{\partial_r \bar{n}_{\text{eq}}}{\bar{n}_{\text{eq}}} + \left( E - \frac{3}{2} \right) \frac{\partial_r \bar{T}_{\text{eq}}}{\bar{T}_{\text{eq}}} \right\}^2 \right\rangle_E$$

- In the limit  $\omega \gg \omega_D$ , gives the same result as fluid equations, including reversal of thermodiffusion sign.

## Passing particles

- Final expression:

$$\partial_t S_{\text{eq}} = \pi \int dV n_{\text{eq}} \sum_{\mathbf{k}\omega} |v_{E,\mathbf{k}\omega}|^2 \left\langle \delta(\omega - \omega_d - \mathbf{k}_{\parallel} v_{T\parallel}) \zeta \left\{ \frac{\partial_r \bar{n}_{\text{eq}}}{\bar{n}_{\text{eq}}} + \frac{1}{2} (\zeta^2 - 1) \frac{\partial_r \bar{T}_{\parallel \text{eq}}}{\bar{T}_{\parallel \text{eq}}} + (\mathbf{h} - 1) \frac{\partial_r \bar{T}_{\perp \text{eq}}}{\bar{T}_{\perp \text{eq}}} + \zeta \left( \frac{\partial_r V_{\parallel \text{eq}}}{v_{T\parallel}} - \frac{\mathbf{k}_{\parallel}}{k_{\theta} \rho_s} \right) \right\}^2 \right\rangle_{\zeta, \mathbf{h}}$$

**Turbulent spin-up** Dominguez & Staebler

93, Diamond et al 94, XG 01, Coppi 02

## Discussion

- Transport matrix satisfies  $D_{nn}D_{TT} - D_{nT}^2 > 0$  (2nd principle).
- Thermodiffusion  $D_{nT}$  changes sign with average fluctuation phase velocity  $\langle \omega/\omega_D - \zeta \rangle$ . Inward particle transport for ITG dominated turbulence.
- Minimum of entropy production corresponds to finite density and temperature gradients: **generalisation of stiffness concept.**
- However a state with zero fluxes such that

$$n_{eq} = n_0 e^{-\frac{2}{R_0} \int_0^r \lambda dr} \quad T_{eq} \propto n_{eq}^{\zeta-1}$$

**is not attainable because it is linearly stable** Angioni 05.



## Discussion (cont.)

- Other pinch mechanisms:
  - inward thermodiffusion of passing electrons due to parallel dynamics - order  $o(\omega/k_{\parallel}V_{Te})$  Jenko 00, Hallatschek 01
  - fractional kinetics Castillo del Negrete 05 or CTRW Van Milligen 04

$$\frac{\partial n(x,t)}{\partial t} = S(x) - \frac{n(x,t)}{\tau_D(x)} + \int_0^1 dx' p(x-x',x';t) \frac{n(x',t)}{\tau_D(x')}$$

$$p\left(x-x'; \frac{dn}{dx}(x';t)\right) = \zeta(x',t) P_{sym}(x-x',1,\sigma_1) + [1 - \zeta(x',t)] P_{sym}(x-x',2,\sigma_2)$$

$$\zeta(x',t) = \Theta \left[ \left| \frac{dn}{dx}(x',t) \right| - \left( \frac{dn}{dx} \right)_{crit} \right]$$

- coupling between passive scalar and vorticity transport  $d_t(n - \nabla^2 \phi) = 0$  Priego 05  $\rightarrow$  clustering of particles in vortical structures.

## Testing theory with the TRB code

- TRB solve 3D fluid equations .
- Same as simplified 2D model + polarization drift and parallel dynamics.
- Neoclassical transport is not included.
- Covers Ion Temperature Gradient / Trapped Electron Mode turbulence.

## Equations solved by the TRB code

$$d_t n_e = -V_{dte} \cdot [\nabla p_e - n_e \nabla \phi] + S_n$$

$$d_t p_e = -\zeta V_{dte} \cdot [\nabla(T_e p_e) - p_e \nabla \phi] + S_{pe}$$

$$d_t \Omega = -n_i \nabla_{//} V_{//i} + [p_i, \nabla^2 \phi] + (1 - f_t)[n_e, \phi] \\ + f_t V_{dte} \cdot [\nabla p_e - n_e \nabla \phi] - V_{di} \cdot [\nabla p_i - n_i \nabla \phi]$$

$$d_t V_{//i} = -n_i \nabla_{//} \phi - \nabla_{//} p_i + S_{V_{//i}}$$

$$d_t p_i = -\zeta V_{di} \cdot [\nabla(T_i p_i) + p_i \nabla \phi] - \zeta p_i \nabla_{//} V_{//i} + S_{pi}$$

$$d_t = \partial_t - \left( \frac{\mathbf{B}}{B^2} \times \nabla \phi \right) \cdot \nabla \quad ; \quad \Omega = n_{e,eq} \left[ \frac{1 - f_t}{T_{e,eq}} (\phi - \langle \phi \rangle) - \nabla^2 \phi \right] \quad ; \quad \zeta = \frac{5}{3}$$

## TRB calculations agrees with QL theory for particle transport

Two additive contributions:

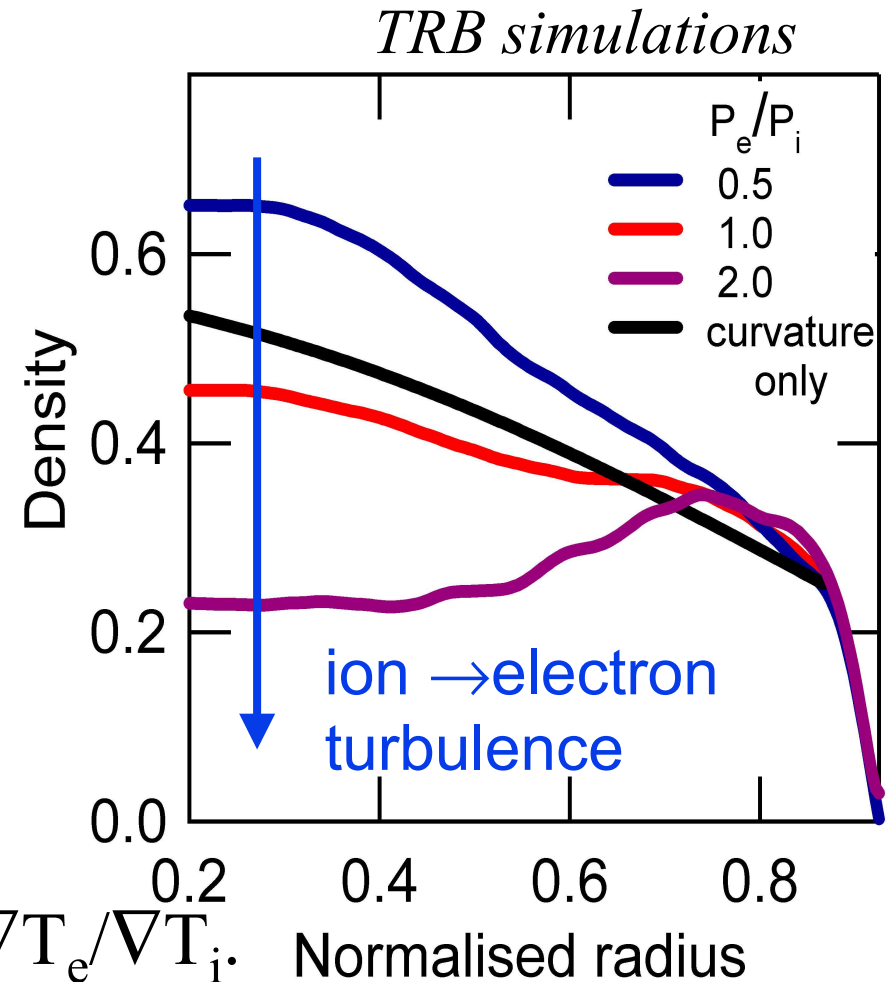
- Curvature pinch, depends on magnetic shear

$$\frac{V}{D} \propto s \quad s = \frac{r}{q} \frac{dq}{dr}$$

- Thermo-diffusion

$$\frac{V}{D} \propto \frac{\nabla T}{T}$$

changes sign when increasing  $\nabla T_e / \nabla T_i$ .



## Impurity transport

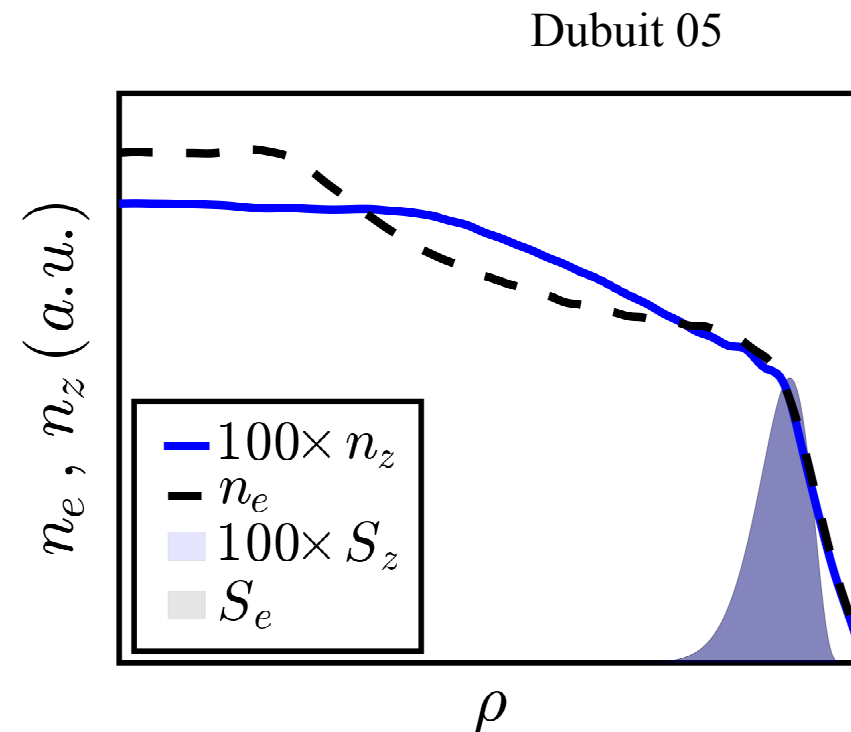
- Issue: is the impurity pinch velocity turbulent or neoclassical?
- Prediction of quasi-linear theory

$$\Gamma_{Z\text{turb}} = -D_Z \left\{ \underbrace{\frac{dn_Z}{dr}}_{\substack{\uparrow \\ \text{Diffusion}}} + C_q(s) \underbrace{\frac{2}{R} n_Z}_{\substack{\uparrow \\ \text{Curvature pinch} \\ \text{inward}}} - C_T(\omega) \underbrace{\frac{dT_Z}{T_Z dr} n_Z}_{\substack{\uparrow \\ \text{Thermodiffusion} \\ \sim 1/Z, \text{ outward} \\ \text{for ion turb.}}} \right\}$$

TRB has been modified to add an impurity Dubuit 05

## Evidence of an inward impurity pinch

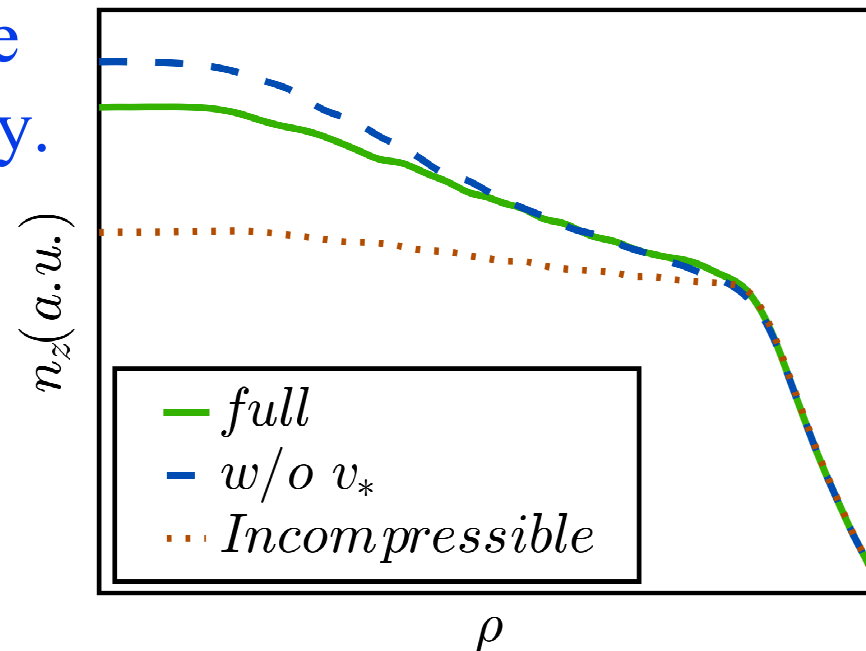
- Both Carbon and electron sources are peripheral.
- Peaked electron and impurity densities → **inward pinch**. Similar to Estrada-Mila 05
- Profiles are different.



## Curvature seems to be the dominant mechanism

- Thermodiffusion and curvature pinches can be switched-off numerically.
- Curvature pinch is dominant.
- Thermodiffusion is directed outward and is small.

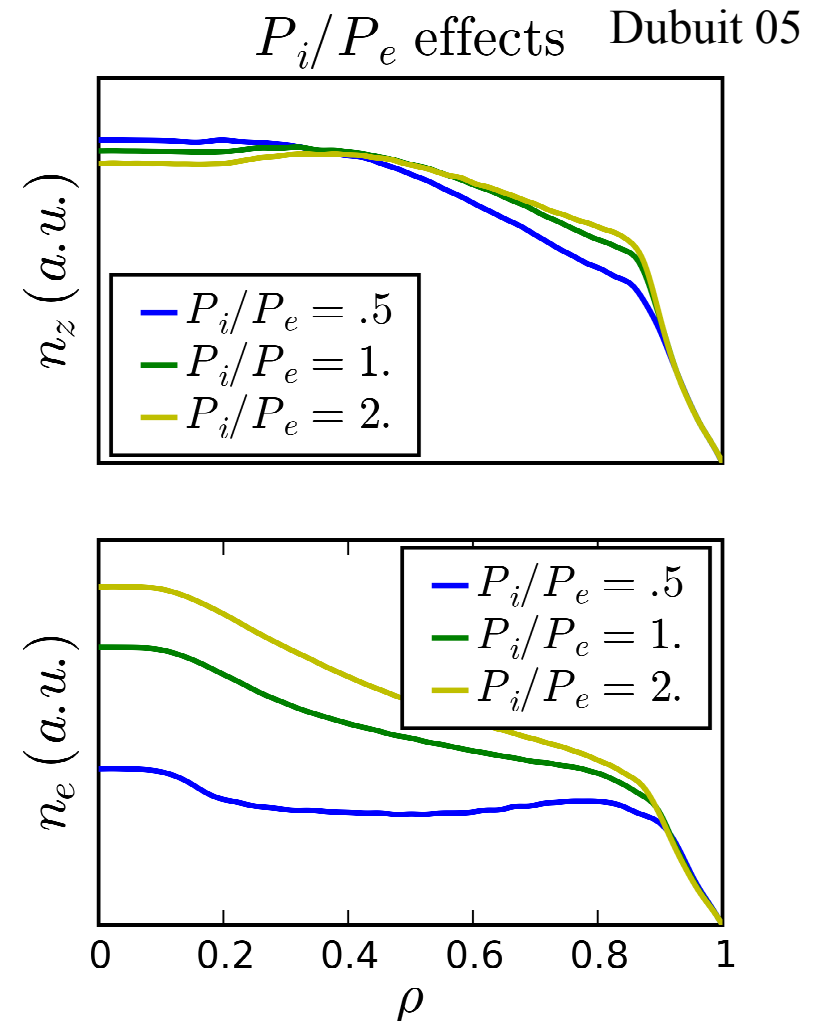
Dubuit 05



- Unexplained small residual contribution

## Effect of $P_e/P_i$

- Increasing the ratio of ion to electron heating sources:
  - electron density profile is more peaked
  - impurity profile is less peaked.
- Consistent with quasi-linear prediction. Estrada-Mila 05, Ongoing comparison with GS2 Angioni 05





## Conclusions

- Curvature pinch is not a thermodynamical force: geometrical effect that leads to **new definitions of density and temperature forces**

$$\bar{n} = n / n_{\text{can}} \quad \bar{T} = T / T_{\text{can}}$$

$$n_{\text{can}} = n_0 I^{-1} \quad ; \quad T_{\text{can}} = T_0 I^{-(\zeta-1)} \quad ; \quad I = \exp\left(\frac{2}{R_0} \int_0^r \lambda dr\right)$$

- **Onsager symmetry is found once this normalisation is done.**
- **Entropy production rate is always positive, within the frame of quasi-linear theory.**

## Conclusions (cont.)

- Some of these predictions have been tested with the TRB code:
  - Particle pinch velocity is the **sum of curvature and thermodiffusion pinches**. Somewhat formal however, except for trace impurities.
  - **Impurity pinch velocity is dominated by curvature pinch.**
  - **For ion turbulence: particle thermodiffusion pinch velocity is inward and impurity pinch velocity is outward.**
- **Collisionality is an issue.**

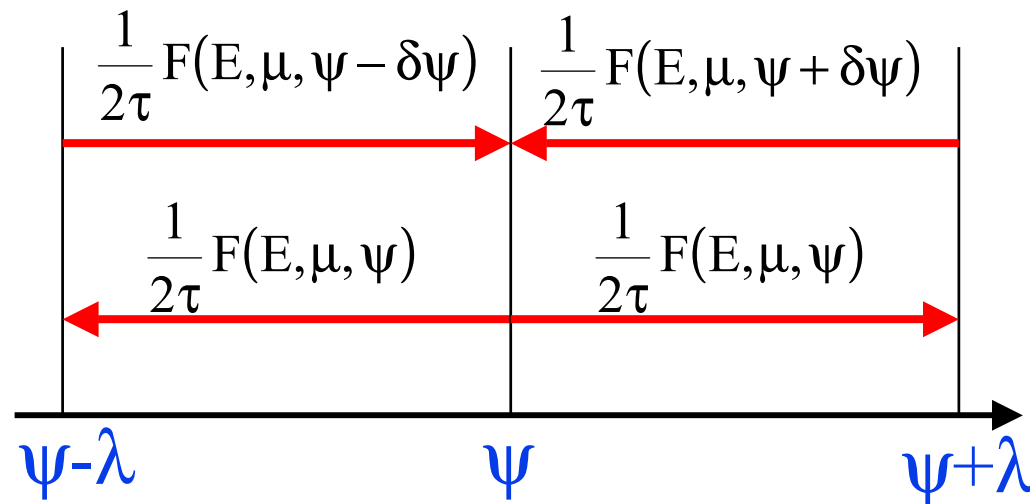
# Transport equations

$$\partial_t \bar{n}_{\text{eq}} + \frac{1}{r} \partial_r (r\Gamma) = 0$$

$$\frac{1}{\zeta - 1} \bar{n}_{\text{eq}} \partial_t \bar{T}_{\text{eq}} + \frac{1}{r} \partial_r (rQ) = -\frac{1}{\zeta - 1} \Gamma \partial_r \bar{T}_{\text{eq}}$$

## Diffusion : conventional model

- Random walk: step size  $\delta\psi$ , time step  $\tau$ , distribution function  $F(E, \mu, \psi, t)$

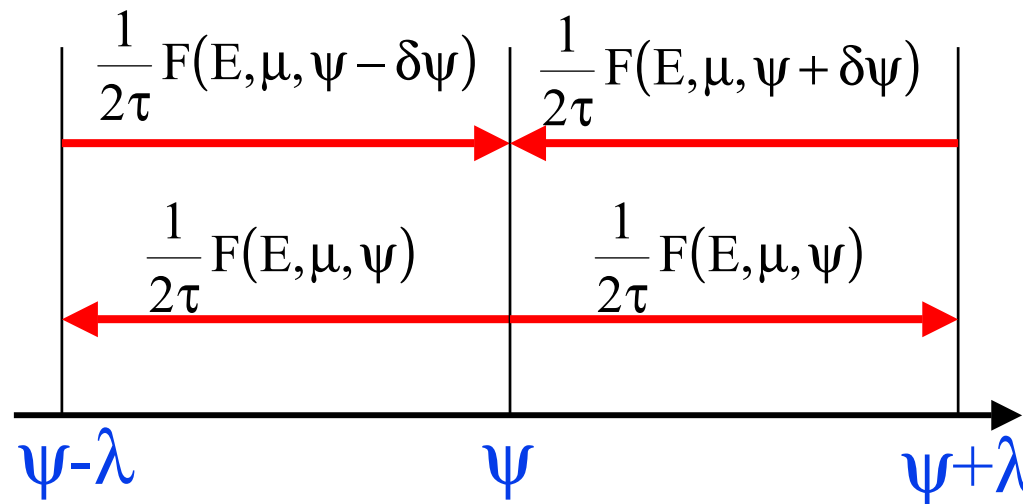


- Particle balance  $\rightarrow$  diffusion equation  $D = \delta\psi^2/2\tau$

$$\partial_t F = D \partial_{\psi\psi} F \quad \rightarrow \quad \partial_t n = D \partial_{\psi\psi} n$$

## Thermodiffusion

- Step size  $\delta\psi$  depends on energy  $E \rightarrow D(E)$ , e.g.  
 $D = D_0 + D_1(E/T - 3/2)$



- Temperature gradient appears in particle flux

$$\partial_t F = D \partial_{\psi\psi} F \quad \rightarrow \quad \partial_t n = \partial_{\psi} \left( D_0 \partial_{\psi} n + D_1 n \frac{\partial_{\psi} T}{T} \right)$$

## Diffusion and pinch velocity

- Particle flux

$$\Gamma_e = -D \frac{dn_e}{dr} + V n_e$$

- Diffusion is turbulent

$$D = D_{\text{turb}}$$

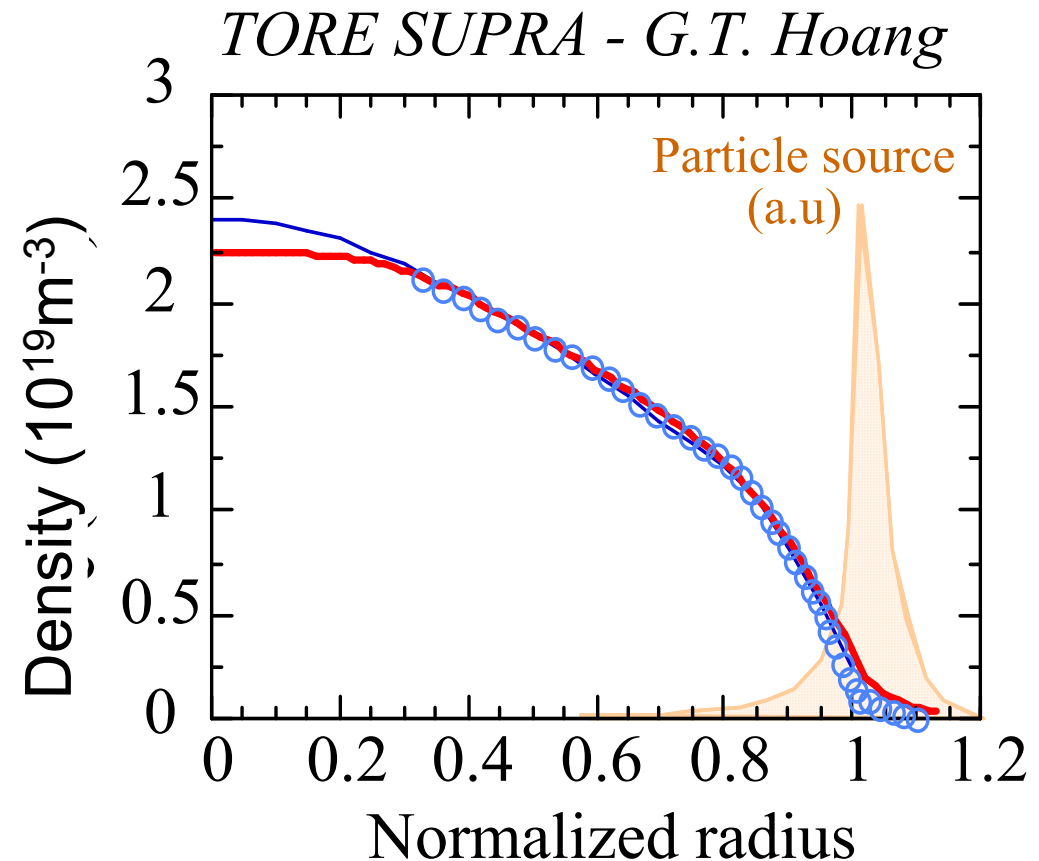
- pinch velocity = collisions + turbulence

$$V = V_{\text{coll}} + V_{\text{turb}}$$

- In a reactor:

- ionisation source localised in the edge  $\rightarrow \Gamma_e = 0$

- $V_{\text{coll}} \sim V_{\text{Ware}} = 0$ . Turbulent pinch  $V_{\text{turb}} \rightarrow$  density peaking?

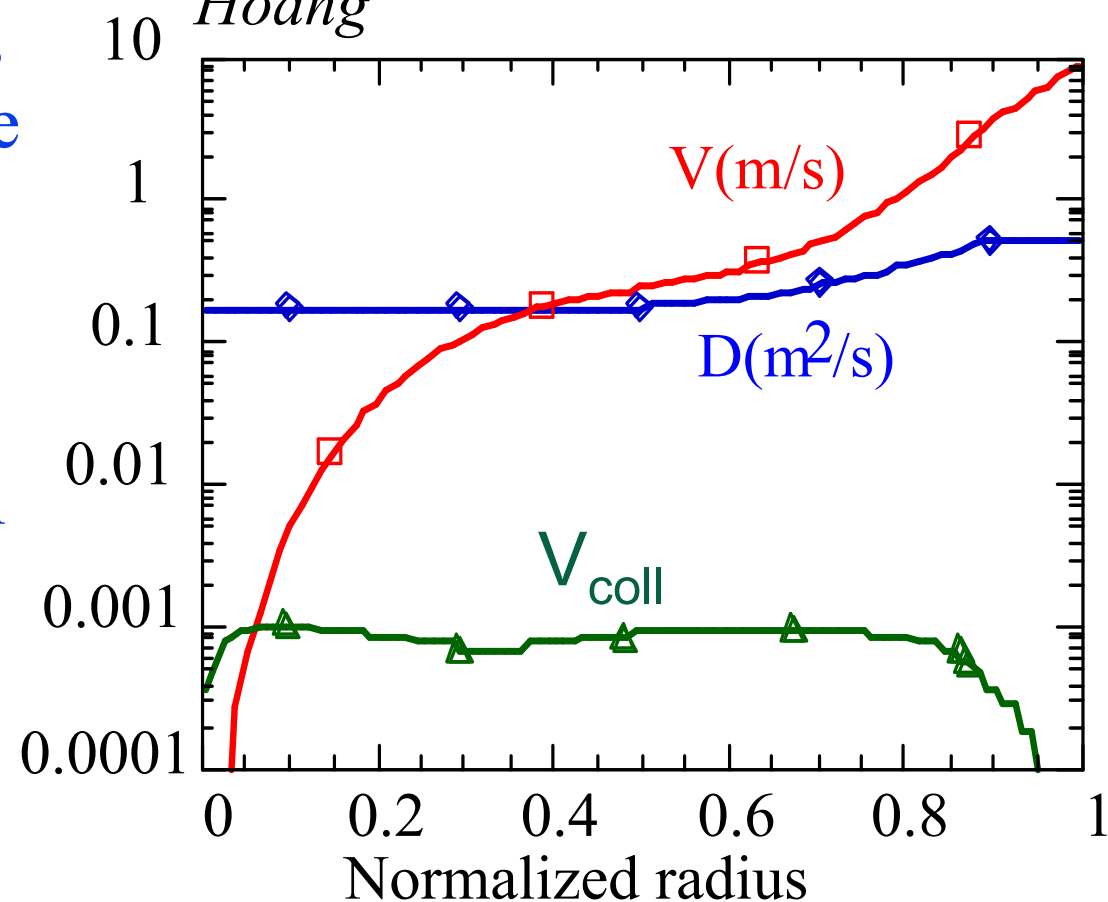


## Pinch is turbulent in L-mode

*Diffusion and pinch velocity vs  
radius - TORE SUPRA - G.T.*

*Hoang*

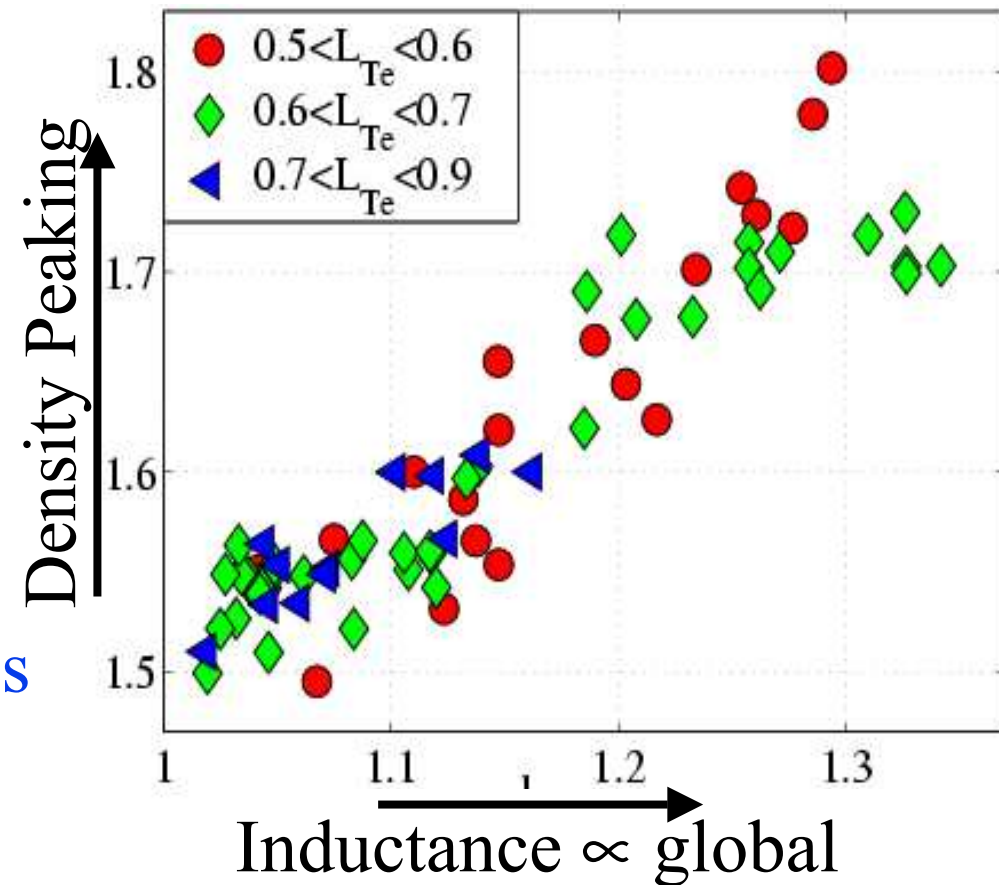
- In TORE SUPRA, and TCV: no Ware pinch,  $V_{\text{Ware}}=0$ .
- Peaked density profile, ionisation source localised in the edge  $\rightarrow$  turbulent pinch velocity.



## Density and safety factor profiles are correlated

- Combined heating and current drive :
  - consistent with curvature pinch
  - no indication of thermodiffusion:
- e/ion-mode transition?
- density and q profiles are correlated in JET, DIID, TCV, TS...

*JET- H. Weisen, A.Zabolotsky*





## Density profiles are peaked at low collisionality

*H. Weisen, A. Zabolotsky*

- $V/D$  decreases with collisionality.
- Consistent with observations on AUG and JET.
- At large collisionality,  
 $V_{\text{turb}} \approx V_{\text{ware}}$   
(*J. Stober, M. Valovic*)

