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EUROfusion

Second order Gyrokinetic theory for Particle-In-Cell codes

Vlasov-Boltzmann equations 2017, CIRM, Marseille, France

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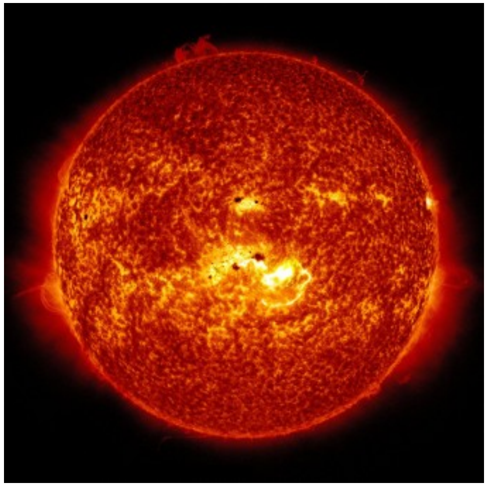
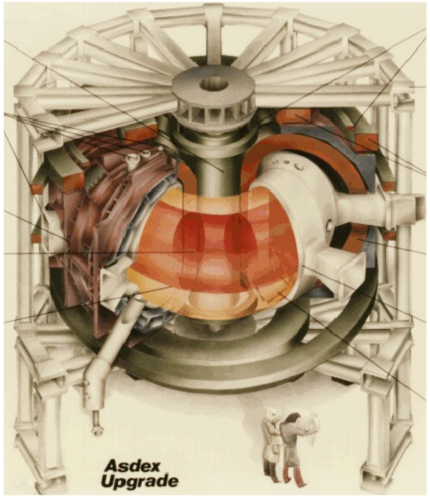
From kinetics to gyrokinetics (GK)



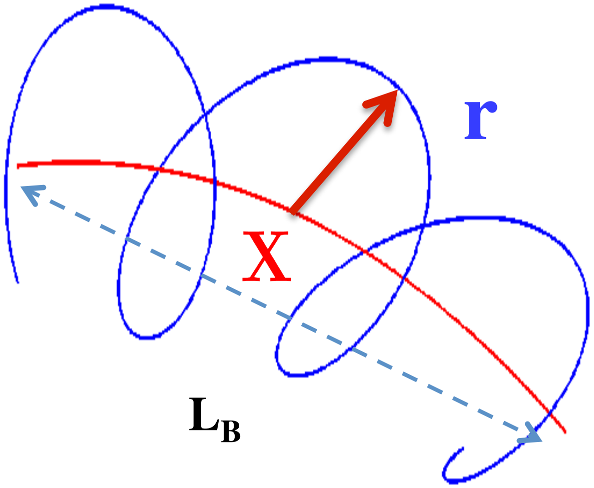
Fusion reaction

$$D - T : He^4(3.5MeV) + n(14MeV)$$

From the Sun to Laboratory



Plasma with strong magnetic field: fusion plasma
Multi-scaled motion of charged particles
θ fast angle (gyroangle)
$\mu = mv_\perp^2/2B$ slow adiabatic invariant



Gyrokinetics: removing the fastest gyro-motion from the dynamical description;
Gain of calculation time

6D (kinetic) (4+1)D (gyrokinetic)

$$(\mathbf{x}, \mathbf{p}) \longrightarrow (\mathbf{X}, p, \mu, \theta)$$

L_B spatial length of magnetic field curvature variation

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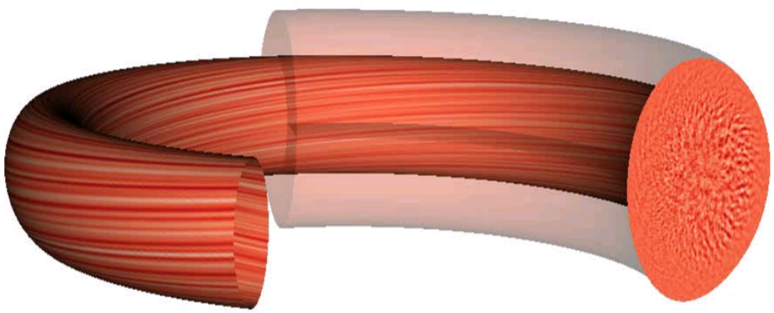
Introduction

- **Gyrokinetic theory: an important theoretical tool for magnetised plasma simulations**
- **An accurate tool for modeling of turbulent transport**:
  major issue for plasma confinement
- Various theoretical nomenclature & orderings :
  different Gyrokinetic (GK) models (set of equations)
- Various numerical implementations **: are the numerical results trustworthy?**

- Most popular numerical implementations
  - **PIC codes (ORB5, EUTERPE etc)**
  - **Vlasov (Eulerian) codes:** grid based (**GENE, GKW**)
  - **Semi-Lagrangian codes (GYSELA)**



Simulation of turbulence in ASDEX Upgrade with ORB5

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VeriGyro: a project on GK code verification

- **GK codes: significant development: global electromagnetic implementations**
  - **Electrostatic gyrokinetic implementations :** theory & simulations: **well established**
  - **Global electromagnetic gyrokinetic implementations:**
    - Next level of complexity: Alfvèn physics
    - A lot of freedom for approximations (Poisson and Ampère equations)
    - **Different codes implement different version of GK equations**
- **Goals:**
  - Building up the general hierarchy of the GK equations implemented numerically
  - **Global electromagnetic** Intercode benchmark

VeriGyro has been
Successfully delivered
2014-2017

- **Focus Today**

ORB5 *[**Jolliet** Comp. Phys. Comm. 2007; **Bottino** PPCF, 2011; **Tronko** Phys. Pl., 2016]*

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GK Orderings

- **Guiding- center:** background quantities: $\epsilon_B = \rho_0 \left|\nabla B/B\right|$
- **Gyrocenter:** fluctuating fields:

$$\epsilon_\delta = (k_\perp \rho_i)\frac{e\delta\phi}{T_i}$$

$$\epsilon_\omega = \frac{\omega}{\Omega_{\text{ci}}}$$

- Anisotropy of turbulence

$$\epsilon_{\|} = k_{\|}/k_\perp \ll 1$$

$$\epsilon_{||} \sim \epsilon_\omega \sim \epsilon_\delta$$

- **Ordering defines physics: There is NO unique gyrokinetic model**

- Gyrokinetics

  $k_\perp \rho_i \sim 1$

- Drift-kinetics

  $k_\perp \rho_i \ll 1$

- Maximal ordering

  $\epsilon_B \sim \epsilon_\delta$

- Code ordering

  $\epsilon_B \ll \epsilon_\delta$

- High β (GENE local)

  $\delta B_{\|}/B \sim \delta B_\perp/B$

- Low β (ORB5)

  $\delta B_{\|}/B \ll \delta B_\perp/B$

[Tronko, Chandre, arXiv:1709.05222, 2017] $\epsilon_B = \epsilon_\delta^2$

[Brizard, Hahm Rev.Mod.Phys., 2007] $\epsilon_B = \epsilon_\delta^{3/2}$

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Gyrokinetic field theory: concept

Particles(GK) dynamical reduction
Goal: remove fastest scale of motion

Gauge transformation & Canonical Lie-Transform

Guiding-center

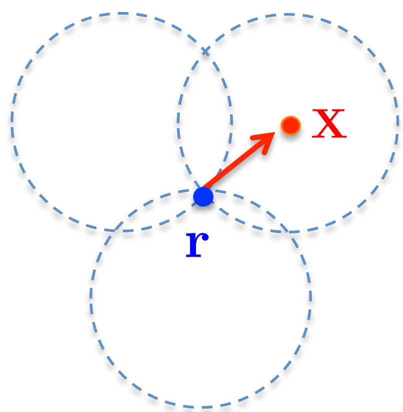
Canonical Lie-Transform

Gyrocenter

Variational principle:

Coupling fields & gyrocenters

Reduced GK Vlasov+ GK Maxwell equations



Bonus: Noether theorem for energy conservation diagnostics

- **Polarization effects: fields and particles are not evaluated at the same position anymore: polarization shifts in GK Ampére and Poisson equations**

Field theory guarantees consistency

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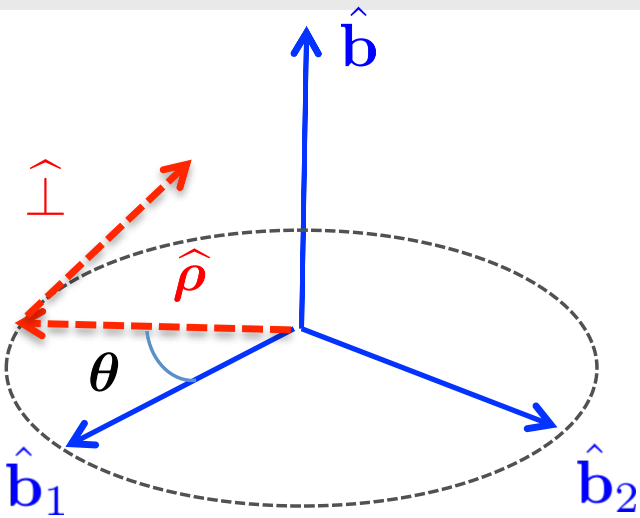
Local particle coordinates



- Non-canonical local particle coordinates 6D:

$$\mathbf{Z}^{\alpha} = (\mathbf{x}, \mathbf{v}) \to \left(\mathbf{x}, v_{\|}, \mu, \theta\right)$$

- Rotating particle basis:

$$\left.\begin{aligned} \widehat{\perp} &= -\widehat{\mathbf{b}}_1 \sin\theta - \widehat{\mathbf{b}}_2 \cos\theta \\ \widehat{\boldsymbol{\rho}} &= \widehat{\mathbf{b}}_1 \cos\theta - \widehat{\mathbf{b}}_2 \sin\theta \end{aligned}\right\}$$

- Magnetic Momentum:
  adiabatic invariant

$$\mu = \frac{m v_{\perp}^2}{2B}$$

- Velocity vector decomposition

$$\mathbf{v} = v_{\|}\widehat{\mathbf{b}} = \mathbf{v}_{\perp} = v_{\|}\widehat{\mathbf{b}} + (2\mu m B)^{1/2}\,\widehat{\perp}$$

- **Goal of the dynamical reduction:** build up a change of variables such that fast gyromotion is uncoupled

$$\dot{\mu} = 0$$

- Relevant dynamics on the reduced (4+1)D phase space:

$$\left(\mathbf{X}, v_{\|}; \mu\right)$$

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Gyrokinetic field theory: ORB5

- **Common framework for code models derivation:** *[Sugama Phys. Pl. 2000]*

$$L = \sum_{\rm sp} \int \mathrm{d}\Omega_0 \; F(\mathbf{Z}_0, t_0) L_p(\mathbf{Z}(\mathbf{Z}_0, t_0; t), \dot{\mathbf{Z}}(\mathbf{Z}_0, t_0; t), t) + \int \mathrm{d}V \frac{|\mathbf{E}_1|^2 - |\mathbf{B}_1|^2}{8\pi}$$

- Phase-space volume $d\Omega = dV\, dW$
- Time-independent: **ORB5**
- **Conserved** $\mathrm{d}\Omega_0 = \mathrm{d}\Omega$

$$\mathbf{Z} = (\mathbf{X}, p_z, \mu, \theta)\,; dW = \frac{2\pi}{m^2} B_\|^* dp_z d\mu$$

$$p_z = m v_\| + \frac{e}{c}\epsilon_\delta A_{1\|} \quad \mathbf{B}^* = \boldsymbol{\nabla} \times \left(\mathbf{A} + \frac{c}{e} p_z \widehat{\mathbf{b}}\right)$$

- Vlasov constraint: Distribution function of species "sp":
- Conserved along the characteristics $F(\mathbf{Z}_0, t_0) = F(\mathbf{Z}, t)$

- Gyrocenter Lagrangian: reduced motion of a single particle (code ordering)

$$L_p = \left(\frac{e}{c}\mathbf{A} + \left(\frac{e}{c}\epsilon_\delta A_{1\|} + m v_\|\right)\widehat{\mathbf{b}}\right) \cdot \dot{\mathbf{X}} + \frac{mc}{e}\mu\dot{\theta} - H$$

- Hamiltonian decomposition

$$H = H_0 + \epsilon_\delta H_1 + \epsilon_\delta^2 H_2$$

- Non-perturbed dynamics $H_0^{\rm ORB5} = \frac{p_z^2}{2m} + \mu B$

- Linear Dynamics

$$H_1^{\rm ORB5} = -e\; \mathcal{J}_0^{\rm gc}\left(\psi_1^{\rm ORB5}\right)$$

$$\psi_1^{\rm ORB5} = \phi_1 - \mathbf{A}_{1\|} p_z / m$$

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Hamiltonian hierarchy: Theory & ORB5

- **Theory: full FLR electromagnetic** Hamiltonian **correspondance to Hahm's 1988 electrostatic model** $\epsilon_\perp = k_\perp \rho_0 = 1$

$$H_{2\mathrm{full}}^{\mathrm{THEORY}} = \frac{e^2}{2mc^2} \mathcal{J}_0^{\mathrm{gc}} \left(\mathbf{A}_{1\|}(\mathbf{X} + \boldsymbol{\rho}_0)^2 \right) - \frac{e^2}{2B} \mathcal{J}_0^{\mathrm{gc}} \left(\frac{\partial}{\partial \mu} \widetilde{\psi}_1^{\mathrm{ORB5}} (\mathbf{X} + \boldsymbol{\rho}_0)^2 \right)$$

$$\psi_1^{\mathrm{ORB5}} = \phi_1 - \mathbf{A}_{1\|} p_z / m$$

Electromagnetic coupling between GK Poisson and Ampère equations

- **Up to the 2nd order FLR truncation : long wavelength approximation** $\epsilon_\perp = k_\perp \rho_0 \ll 1$

$$H_2^{\mathrm{FLR}} = \frac{e^2}{2mc^2} A_{1\|}(\mathbf{X})^2 + \frac{\mu}{2B} \left| \boldsymbol{\nabla}_\perp A_{1\|}(\mathbf{X}) \right|^2 + \frac{1}{2} \frac{\mu}{B} A_{1\|} \boldsymbol{\nabla}_\perp^2 A_{1\|}(\mathbf{X}) - \frac{mc^2}{2B^2} \left| \boldsymbol{\nabla}_\perp \phi_1(\mathbf{X}) - \frac{p_z}{mc} A_{1\|}(\mathbf{X}) \right|^2$$

- **ORB5 up to the 2nd order FLR: truncation of semi-electromagnetic** $H_{2\mathrm{full}}^{\mathrm{ORB5}}$

$$\epsilon_\perp = k_\perp \rho_0 \ll 1 \qquad \beta \ll 1$$

$$H_2^{\mathrm{ORB5}} = \frac{e^2}{2mc^2} A_{1\|}(\mathbf{X})^2 + \frac{\mu}{2B} \left| \boldsymbol{\nabla}_\perp A_{1\|}(\mathbf{X}) \right|^2 + \frac{1}{2} \frac{\mu}{B} A_{1\|} \boldsymbol{\nabla}_\perp^2 A_{1\|}(\mathbf{X}) - \frac{mc^2}{2B^2} \left| \boldsymbol{\nabla}_\perp \phi_1(\mathbf{X}) \right|^2$$

Uncoupled GK Poisson and Ampère equations

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How to build up a GK model consistently?

- All approximations **should** be performed on the Lagrangian L **before** deriving the equations of motion:
  - Approach guarantees energetic consistency of final equations
  - Symmetry properties of Lagrangian are automatically transferred to the equations
  - **Significant numerical advantage:** Use conserved quantities for building code diagnostics: ORB5 new physics of electromagnetic microinstabilities

- **Set up polarization effects into the system (choose from hierarchy of models):**
  - **Choice of the second order gyrocenter Hamiltonian defines reduced field- particles dynamics**

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Quasi-neutrality approximation

- **Electrostatic contributions from fields and gyrocenter polarization:**
- **Example: ORB5 long-wavelength**

$$\int dV \frac{|\mathbf{E}_1|^2}{8\pi} + \int d\Omega\ F\ \frac{mc^2}{2B^2}\left|\boldsymbol{\nabla}_\perp\phi_1\right|^2 = \frac{1}{8\pi}\int dV\ \left(1+\frac{\rho_s^2}{\lambda_d^2}\right)\left|\boldsymbol{\nabla}_\perp\phi_1\right|^2$$

- **Comparing the Electric field energy: Maxwell's field term & the polarization from the second order particle dynamics**

$$H_2^{\mathrm{ORB5}} = \frac{e^2}{2mc^2}A_{1\|}(\mathbf{X})^2 + \frac{\mu}{2B}\left|\boldsymbol{\nabla}_\perp A_{1\|}(\mathbf{X})\right|^2 + \frac{1}{2}\frac{\mu}{B}A_{1\|}\boldsymbol{\nabla}_\perp^2 A_{1\|}(\mathbf{X}) - \frac{mc^2}{2B^2}\left|\boldsymbol{\nabla}_\perp\phi_1(\mathbf{X})\right|^2$$

$$\lambda_d^2 = \frac{k_B T_e}{4\pi n e^2}$$

Debye length

$$k_\perp\rho_0 \ll 1$$

$$\rho_s^2 = \frac{k_B T_e m c^2}{e^2 B^2}$$

Sound ion Larmor radius

$$\frac{\rho_s^2}{\lambda_d^2} = \frac{4\pi n m c^2}{B^2} = \frac{c^2}{v_A^2} \gg 1$$

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Linearised polarization approximation: ORB5

- **Quasi-neutrality approximated Lagrangian**

$$L = \sum_{\rm sp} \int dV\ dW \left(\dot{\mathbf{X}} + \frac{mc}{e}\mu\dot{\theta} - H \right)\ F - \int dV\ \frac{\left|\boldsymbol{\nabla} \times \mathbf{A}_1\right|^2}{8\pi}$$

- **Towards Poisson and Ampère equations with linearised polarization:**

- **Hamiltonian decomposition**

$$H = H_0 + \epsilon_\delta H_1 + \epsilon_\delta^2 H_2$$

- Linear dynamical $\left(H_0 + \epsilon_\delta H_1\right) F$
- Nonlinear non-dynamical $\epsilon_\delta^2 H_2^{\rm ORB5} F_0$

- **Low-β approximation**

$$|B_\perp| = \left|\boldsymbol{\nabla}_\perp A_{1\|}\right|$$

- **Long-wavelength approximation** $\epsilon_\delta^2 H_2^{\rm ORB5} F_0$
- **Semi-electromagnetic full FLR** $\epsilon_\delta^2 H_{\rm 2full}^{\rm ORB5}\ F_0$

- Up to $\sim \mathcal{O}\left(\epsilon_\delta^2\right)$

$$L = \sum_{\rm sp} \int d\Omega \left(\dot{\mathbf{X}} + \frac{mc}{e}\mu\dot{\theta} - \left(H_0 + \epsilon_\delta H_1\right) \right)\ F - \epsilon_\delta^2 \sum_{\rm sp} \int d\Omega\ H_2^{\rm ORB5} F_0 - \epsilon_\delta^2 \int dV\ \frac{\left|\boldsymbol{\nabla}_\perp \mathbf{A}_{1\|}\right|^2}{8\pi}$$

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Linearised GK Field equations: ORB5

- Phase space volume $$d\Omega = dV\ dW$$

- **Polarization equation in a weak form**

$$\frac{\delta L}{\delta \phi_1} \circ \widehat{\phi}_1 = 0$$

- Test function

$$\widehat{\phi}_1 = \phi_1$$

$$\epsilon_\delta \sum_{\text{sp}} \int d\Omega\ F_0\ \frac{mc^2}{B^2} \left|\boldsymbol{\nabla}_\perp \phi_1\right|^2 = \sum_{\text{sp}} \int d\Omega\ \mathcal{J}_0^{\text{gc}} \left(\phi_1\right) \left(F_0 + \epsilon_\delta F_1\right)$$

- **Ampère's equation in a weak form**

$$\frac{\delta L}{\delta A_{1\|}} \circ \widehat{A}_{1\|} = 0$$

- Test function

$$\widehat{A}_{1\|} = A_{1\|}$$

$$\int dV\ \frac{1}{4\pi} \left|\boldsymbol{\nabla}_\perp A_{1\|}\right|^2 + \epsilon_\delta \sum_{\text{sp}} \int d\Omega \frac{e^2}{mc^2} \left(\mathcal{J}_0^{\text{gc}} A_{1\|}\right)^2 F_0 = \sum_{\text{sp}} \int d\Omega \frac{p_z}{mc} \mathcal{J}_0^{\text{gc}} \left(A_{1\|}\right) \left(F_0 + \epsilon_\delta F_1\right)$$

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GK Vlasov equation: ORB5

- **Vlasov equation is reconstructed from the characteristics**

$$\frac{\delta L}{\delta \mathbf{Z}} = 0$$

$$\mathbf{Z} = (\mathbf{X}, p_z, \mu)$$

$$\dot{\mathbf{X}} = \frac{\partial (H_0 + \epsilon_\delta H_1)}{\partial p_z} \frac{\mathbf{B}^*}{B^*_\parallel} - \frac{c}{eB^*_\parallel} \widehat{\mathbf{b}} \times \boldsymbol{\nabla} (H_0 + \epsilon_\delta H_1)$$

$$\dot{p}_z = -\frac{\mathbf{B}^*}{B^*_\parallel} \cdot \boldsymbol{\nabla} (H_0 + \epsilon_\delta H_1)$$

$$\frac{d}{dt} f \left(\mathbf{Z}[\mathbf{Z}_0, t_0, t]; t\right) = \frac{\partial}{\partial t} f\left(\mathbf{Z}, t\right) + \frac{d\mathbf{Z}}{dt} \cdot \frac{\partial}{\partial \mathbf{Z}} f(\mathbf{Z}, t)$$

- **δf model requiers linearized characteristics : only H_0 and H_1**
- **Full-f (nonlinear) model require H_2 contributions in the characteristics**

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Electromagnetic J.E diagnostics

- Noether theorem $\mathcal{E} = \mathcal{E}_k + \mathcal{E}_F$

$$\mathcal{E}_k = \sum_{\rm sp} \int d\Omega \left(\frac{p_z^2}{2m} + \mu B \right) (F_0 + \epsilon_\delta F_1)$$

$$\mathcal{E}_F = \frac{1}{2} \sum_{\rm sp} \int d\Omega \, (F_0 + \epsilon_\delta F_1) \left[\phi_1 - \frac{e p_z}{mc} A_{1\|} \right]$$

- Growth rate measure

$$\gamma = \frac{1}{2\mathcal{E}_F} \frac{d\mathcal{E}_k}{dt} = -\frac{1}{2\mathcal{E}_F} \frac{d\mathcal{E}_F}{dt}$$

$$\frac{d\mathcal{E}_k}{dt} = \sum_{\rm sp} \int d\Omega (F_0 + \epsilon_\delta F_1) \boldsymbol{\nabla} \mathcal{J}_0^{\rm gc} (\phi_1 - \frac{e p_z}{mc} A_{1\|}) \cdot (\mathbf{v}_\| + \mathbf{v}_{\boldsymbol{\nabla} P} + \mathbf{v}_{\boldsymbol{\nabla} B})$$

$$- \sum_{\rm sp} \int d\Omega (F_0 + \epsilon_\delta F_1) \boldsymbol{\nabla} \mathcal{J}_0^{\rm gc} \left(\frac{e p_z}{mc} A_{1\|} \right) \cdot \left[\mu B \boldsymbol{\nabla} \cdot \widehat{\mathbf{b}} + \frac{\mu c}{e B_\|^*} p_z \widehat{\mathbf{b}} \times \left(\widehat{\mathbf{b}} \times \frac{\boldsymbol{\nabla} \times \mathbf{B}}{B} \right) \cdot \boldsymbol{\nabla} B \right]$$

- Electromagnetic simulations: while β increases $\mathcal{E}_F = 0$ $\beta = 0.1\%$
  Mode changes signature: Electromagnetic ITG with KBM destabilizing mechanism
- Real bifurcation from ITG to KBM at $\beta = 1.378\%$

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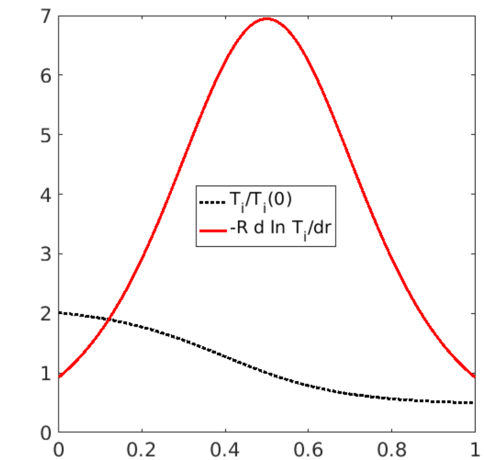
Profiles. Cyclone Base Case

- Common framework for benchmark: *[**Dimits**, Phys. Pl. 2000]*

electrostatic simulations, adiabatic electrons



- The original discharge DIII-D:

H- mode shot #81499 at t=4000 ms;

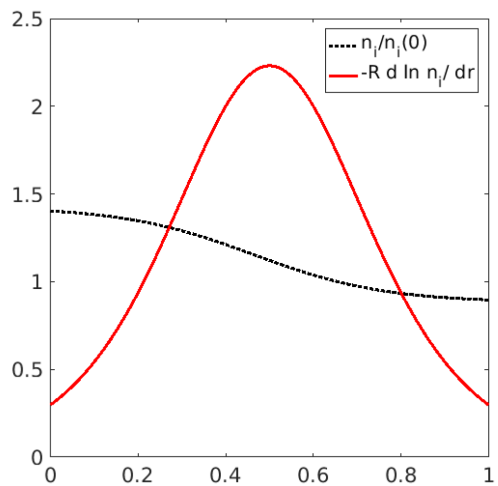
flux tube label r=0.5a

$$q(r) = 0.86 - 0.16(r/a) + 2.52(r/a)^2$$

$$A(r) = A(r_0)\exp\left[-\kappa_A a \Delta A \tanh\left(\frac{r-r_0}{\Delta A a}\right)\right]$$

$$\Delta T_i = \Delta n = 0.3$$

$$\kappa_{T_i} = 6.96 \qquad \kappa_n = 2.23 \qquad T_e/T_i = 1$$



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E_F diagnostics: New effects of electromagnetic microinstabilities

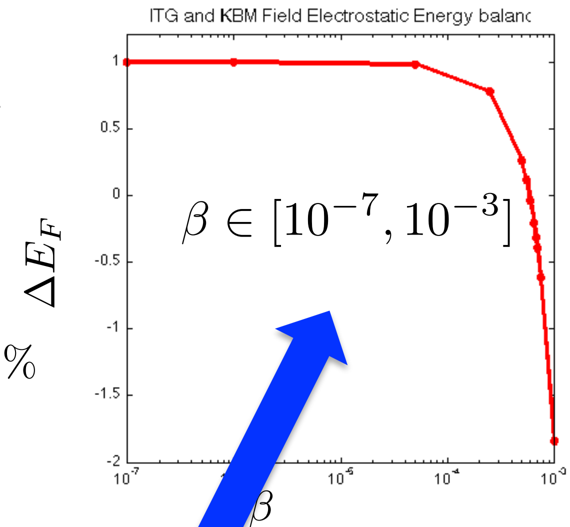
$$\Delta E_{\mathrm{F}} = \frac{E_{\mathrm{F;ES}} - E_{\mathrm{F;EM}}}{E_{\mathrm{F;ES}}}$$

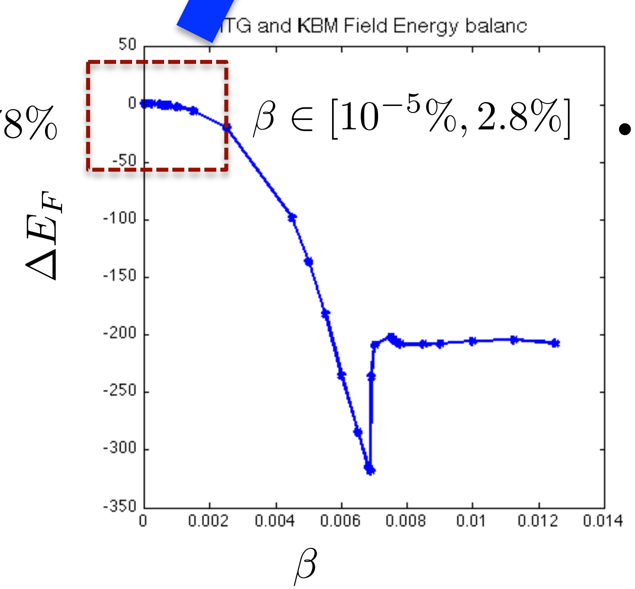
$$\Delta E_F(\beta) = 0 \Rightarrow \beta = 0.1\%$$

Change of destabilizing mechanism: ITG to KBM

$$\min \Delta E_F(\beta) \Rightarrow \beta = 1.378\%$$

ITG to KBM bifurcation





$$\mathcal{E}_F = \frac{1}{2}\sum_{\mathrm{sp}} \int d\Omega \; (F_0 + \epsilon_\delta F_1) \left[\phi_1 - \frac{e p_z}{mc} A_{1\|}\right]$$

- Electrostatic component of field energy

$$E_{\mathrm{F;ES}} = \frac{1}{2}\sum_{\mathrm{sp}} \int d\Omega \; (F_0 + \epsilon_\delta F_1) \; \phi_1$$

- Electromagnetic component of field energy

$$E_{\mathrm{F;EM}} = \frac{1}{2}\sum_{\mathrm{sp}} \int d\Omega \; (F_0 + \epsilon_\delta F_1) \; \frac{e p_z}{mc} A_{1\|}$$

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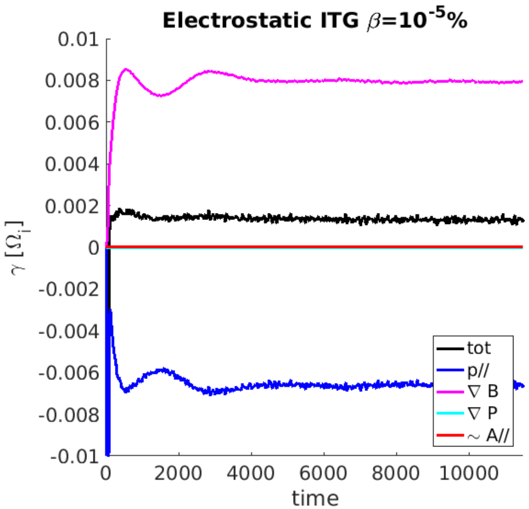
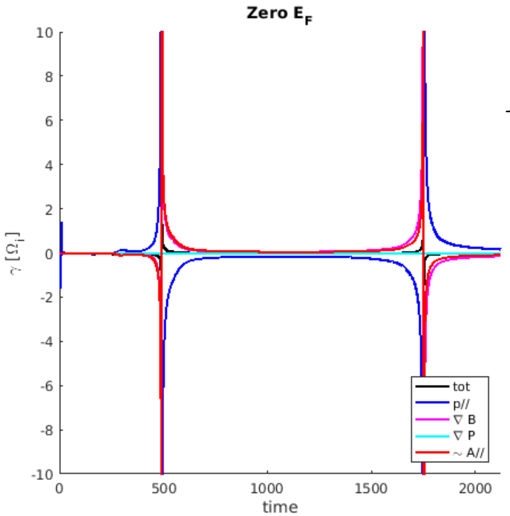
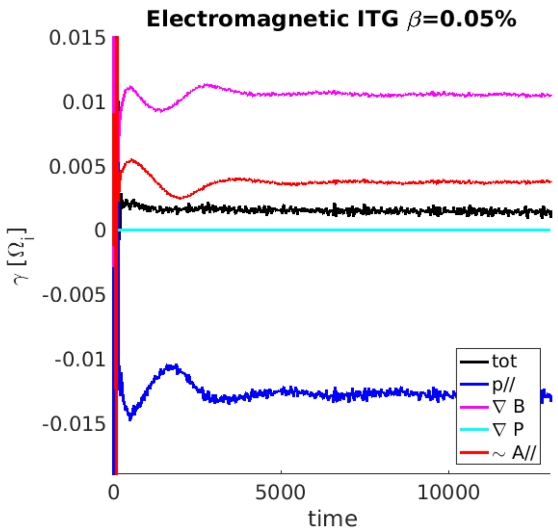
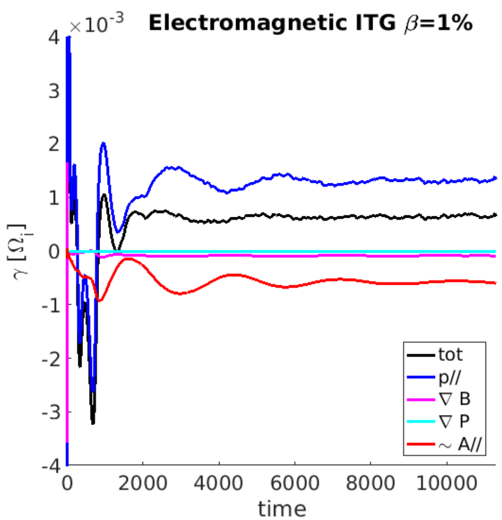
Linear electromagnetic simulations: kinetic electrons





$E_{\mathrm{F;ES}} = 0$





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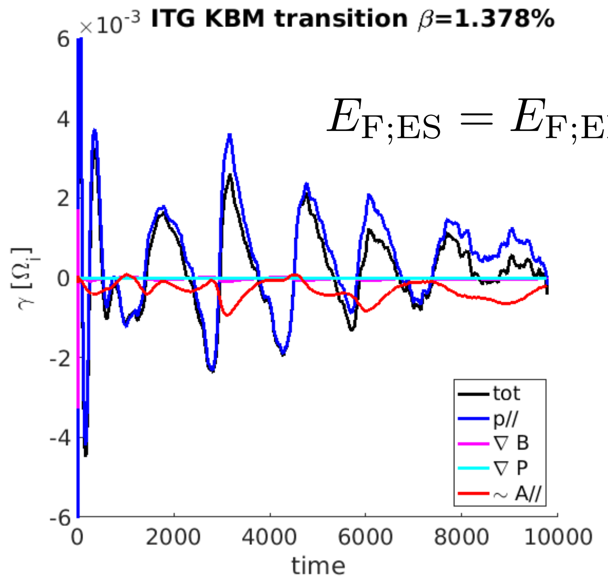
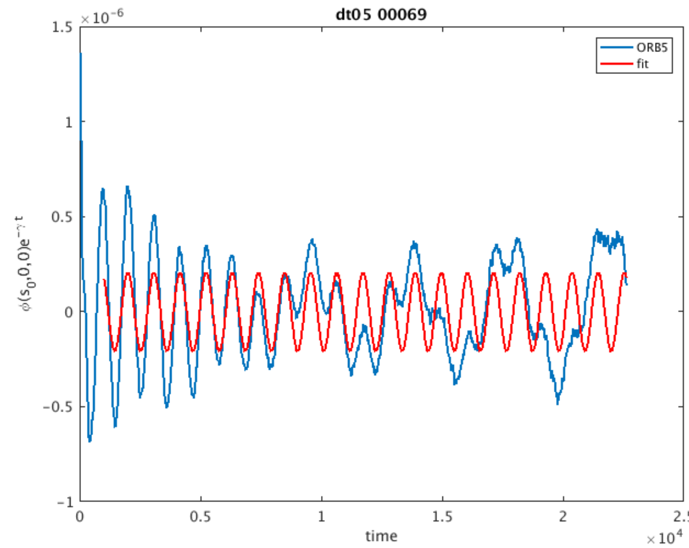
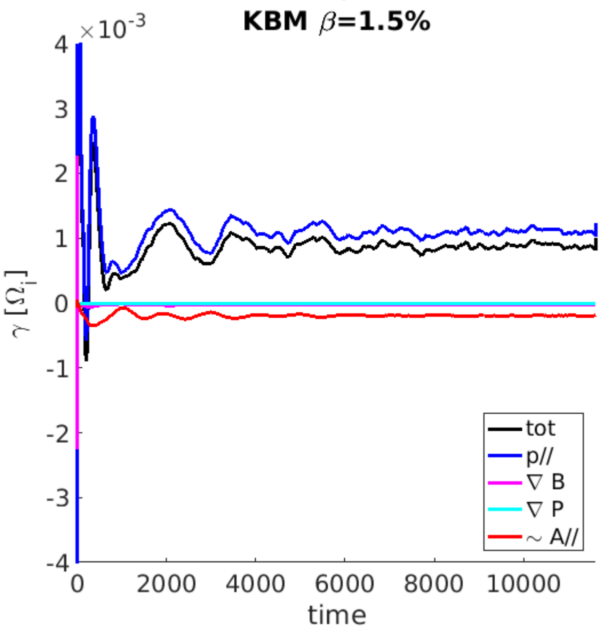
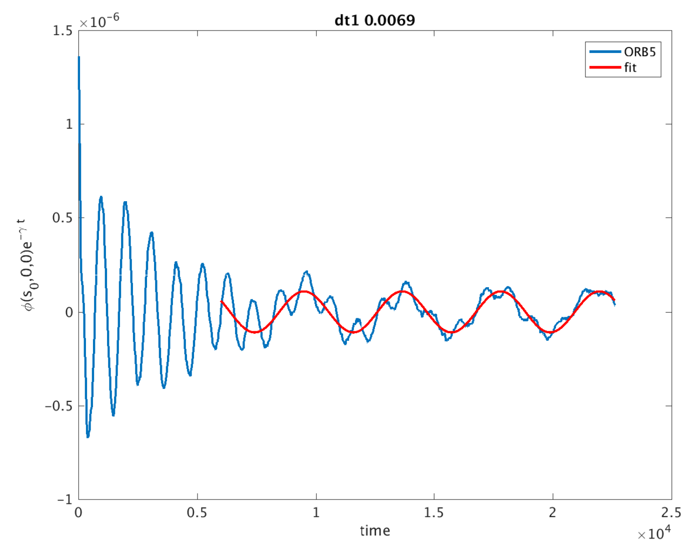
ITG to KBM transition









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Guiding-center dynamical reduction

- **Charged particle; magnetic field** $\gamma = \left(\frac{e}{\epsilon c}\mathbf{A}(\mathbf{x}) + m\mathbf{v}\right)\cdot \mathrm{d}\mathbf{x} - H\mathrm{d}t.$

$H = \frac{m\mathbf{v}^2}{2}$

$\epsilon = \frac{c}{e}$ **Northrop 1960**

Formal parameter proportional to inverse of the amplitude of magnetic field

- **Particle position : instantaneous rotation center and Larmor radius** $\mathbf{x} = \bar{\mathbf{x}} + \boldsymbol{\rho}_0$

  - **Exact solution in SLAB geometry Exists**

$$\epsilon_B = \rho_0 \left|\frac{\boldsymbol{\nabla} B}{B}\right| \sim \rho_i\rho_j \left|\partial^2\mathbf{A}/\partial\bar{x}_i\partial\bar{x}_j\right|$$

- **Real physical ordering: with respect to curvature of magnetic field**

$$\mathbf{w} = \mathbf{v} + \frac{e}{\epsilon m c}\left[\mathbf{A}(\bar{\mathbf{x}} + \boldsymbol{\rho}_0) - \mathbf{A}(\bar{\mathbf{x}}) - (\boldsymbol{\rho}_0\cdot\nabla)\mathbf{A}(\bar{\mathbf{x}}) - \frac{1}{2}(\boldsymbol{\rho}_0\boldsymbol{\rho}_0 : \nabla\nabla)\mathbf{A}(\bar{\mathbf{x}})\right]$$

Infinithesimal shift in velocity $\sim \mathcal{O}(\epsilon_B^2)$

$$\mathbf{w} = w_{||}\hat{\mathbf{b}}(\mathbf{x}) + w_\perp\hat{\perp}(\theta, \mathbf{x})$$

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Guiding-center gauge transformation

$$\gamma = \gamma_0 + \gamma_1 + \mathrm{d}\sigma_1 + \sum_{i=2}^{4} \mathrm{d}\sigma_i + \mathcal{O}(\epsilon_B^2)$$

[Littlejohn 1983]

- **Symplectic part free from oscillations**
- **Hamiltonian**

$$\gamma_0 = \left(\frac{e}{\epsilon c}\mathbf{A}(\bar{\mathbf{x}}) + m w_\| \hat{\mathbf{b}}(\bar{\mathbf{x}})\right) \cdot \mathrm{d}\bar{\mathbf{x}} - H \mathrm{d}t$$

$$H = m w_\|^2/2 + m w_\perp^2/2$$

- **Oscillating part we aim to eliminate up to the second order in** ϵ_B

$$\gamma_1 = \left(\boxed{\frac{e}{\epsilon c}(\boldsymbol{\rho}_0 \cdot \nabla)\mathbf{A}} + \frac{e}{2\epsilon c}(\boldsymbol{\rho}_0\boldsymbol{\rho}_0 : \nabla\nabla)\mathbf{A} + \boxed{m w_\perp \hat{\mathbf{\perp}}(\theta, \bar{\mathbf{x}} + \boldsymbol{\rho}_0)} + m w_\| [\hat{\mathbf{b}}(\bar{\mathbf{x}} + \boldsymbol{\rho}_0) - \hat{\mathbf{b}}(\bar{\mathbf{x}})]\right) \cdot \mathrm{d}\bar{\mathbf{x}}$$
$$+ \left(\frac{e}{\epsilon c}\mathbf{A} + \frac{e}{\epsilon c}(\boldsymbol{\rho}_0 \cdot \nabla)\mathbf{A} + \frac{e}{2\epsilon c}(\boldsymbol{\rho}_0\boldsymbol{\rho}_0 : \nabla\nabla)\mathbf{A} + m w_\perp \hat{\mathbf{\perp}}(\theta, \bar{\mathbf{x}} + \boldsymbol{\rho}_0) + m w_\| \hat{\mathbf{b}}(\bar{\mathbf{x}} + \boldsymbol{\rho}_0)\right) \cdot \mathrm{d}\boldsymbol{\rho}_0.$$

- **physical ordering in** ϵ_B

- **First gauge transformation** $\sigma_1 = -\frac{e}{\epsilon c}\mathbf{A} \cdot \boldsymbol{\rho}_0 - \frac{e}{2\epsilon c}(\boldsymbol{\rho}_0 \cdot \nabla)\mathbf{A} \cdot \boldsymbol{\rho}_0 - \frac{e}{6\epsilon c}(\boldsymbol{\rho}_0\boldsymbol{\rho}_0 : \nabla\nabla)\mathbf{A} \cdot \boldsymbol{\rho}_0$

- **Defining Larmor radius, eliminating** $\mathcal{O}(\epsilon_B^0)$ **oscillating terms**

$$\boxed{\boldsymbol{\rho}_0 = \epsilon \frac{m w_\perp c}{eB} \hat{\boldsymbol{\rho}}}$$

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Guiding-center gauge transformation

- **Near identity coordinate transformation**

$$\bar{\mathbf{x}} = \mathbf{X} + \boldsymbol{\xi}(\mathbf{X}, W_\parallel, W_\perp, \Theta)$$
$$w_\parallel = W_\parallel + \mathcal{W}_\parallel(\mathbf{X}, W_\parallel, W_\perp, \Theta)$$
$$w_\perp = W_\perp + \mathcal{W}_\perp(\mathbf{X}, W_\parallel, W_\perp, \Theta)$$
$$\theta = \Theta + \mathcal{T}(\mathbf{X}, W_\parallel, W_\perp, \Theta)$$

$$\boldsymbol{\xi} \sim \mathcal{W}_\parallel \sim \mathcal{W}_\perp \sim \mathcal{T} \sim \mathcal{O}(\epsilon_B)$$

- **Gauge transformation defines Θ-independent symplectic form and new coordinates**

$$\Gamma = \gamma_0^{\mathrm{sympl}} + \gamma_1 + \mathrm{d}\sigma_1 + \mathrm{d}\sigma_2 + \mathrm{d}\sigma_3 + \mathrm{d}\sigma_4 = \left[\frac{e}{\epsilon c}\mathbf{A}(\mathbf{X}) + mW_\parallel \hat{\mathbf{b}}(\mathbf{X}) - \epsilon\frac{mc}{e}\mu\mathbf{R}\right]\cdot \mathrm{d}\mathbf{X} + \epsilon\frac{mc}{e}\mu \mathrm{d}\Theta$$

$$\sigma_2 = -\frac{e}{\epsilon c}\mathbf{A}\cdot\boldsymbol{\xi}$$

$$\mathbf{R} = \nabla\hat{\mathbf{b}}_1 \cdot \hat{\mathbf{b}}_2 \quad \sim \mathcal{O}(\epsilon_B)$$

$$\sigma_3 = -mW_\parallel \hat{\mathbf{b}}\cdot\boldsymbol{\xi} - \epsilon\frac{m^2 W_\perp^2 c}{2eB}\mathcal{T}$$

$$\mu = \frac{mW_\perp^2}{2B^2}$$

$$\sigma_4 = -\epsilon^2\frac{m^3c^2}{4e^2B^2}W_\parallel W_\perp^2\left[(\hat{\boldsymbol{\rho}}\cdot\nabla)\hat{\mathbf{b}}\cdot\hat{\boldsymbol{\rho}} + (\hat{\perp}\cdot\nabla)\hat{\mathbf{b}}\cdot\hat{\perp}\right]$$

- **Hamiltonian steel being Θ-dependent therefore final coordinate change is required**

$$H = \frac{1}{2}mW_\parallel^2 + \frac{1}{2}mW_\perp^2 + m(W_\parallel\mathcal{W}_\parallel + W_\perp\mathcal{W}_\perp) + \mathcal{O}(\epsilon_B^2)$$

Θ-dependent

Last step: canonical Lie-transform on Hamiltonian to remove Θ-dependency

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Canonical Guiding-center Lie transform

- **Formal scales separation in the Poisson bracket**

$$\{F,G\}_{\rm gc} = \epsilon^{-1}\{F,G\}_{-1} + \{F,G\}_0 + \epsilon\{F,G\}_1$$

- **Canonical Lie-transform (infinitesimal transformation)**

$$\bar{H}(\mathbf{z}) = \mathrm{e}^{-\pounds_S} H(\mathbf{Z}) = H - \{S,H\}_{\rm gc} + \frac{1}{2}\{S,\{S,H\}_{\rm gc}\}_{\rm gc} + \mathcal{O}(S^3)$$

- **Coordinate transform is constructed simultaneously**

$$\mathbf{z} = \mathrm{e}^{\pounds_S}\mathbf{Z} \quad \Rightarrow \quad \begin{aligned} \bar{\mathbf{x}} &= \mathbf{X} + \boldsymbol{\xi} + \{S,\mathbf{X}\}_{\rm gc} \\ w_\| &= W_\| + \mathcal{W}_\| + \{S,W_\|\}_{\rm gc} \\ w_\perp &= W_\perp + \mathcal{W}_\perp + \{S,W_\perp\}_{\rm gc} \\ \theta &= \Theta + \mathcal{T} + \{S,\Theta\}_{\rm gc}, \end{aligned}$$

- **Scalar invariance** $\bar{H}(\mathbf{z}) = H(\mathbf{Z})$

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Guiding-center Poisson bracket

- **Inverting the symplectic matrix**

$$\omega = \mathrm{d}\Gamma = \omega_{ij}\mathrm{d}z^i \wedge \mathrm{d}z^j \quad \Rightarrow \quad \{F,G\}_{\mathrm{gc}} = \frac{\partial F}{\partial z^i}(\omega^{-1})^{ij}\frac{\partial G}{\partial z^j}$$

$$\{F,G\}_{\mathrm{gc}} = \frac{e}{\epsilon mc}\left(\frac{\partial F}{\partial \Theta}\frac{\partial G}{\partial \mu} - \frac{\partial F}{\partial \mu}\frac{\partial G}{\partial \Theta}\right) + \frac{\mathbf{B}^*}{mB_\parallel^*}\cdot\left(\nabla F\frac{\partial G}{\partial W_\parallel} - \frac{\partial F}{\partial W_\parallel}\nabla G\right) - \epsilon\frac{c\hat{\mathbf{b}}}{eB_\parallel^*}\cdot(\nabla F \times \nabla G)$$

- **Symplectic magnetic field**

$$\mathbf{B}^* = \mathbf{B} + \epsilon\frac{mc}{e}W_\parallel \nabla\times\hat{\mathbf{b}} - \epsilon^2\frac{mc^2}{e^2}\mu\nabla\times\mathbf{R} \qquad \mu = \frac{mW_\perp^2}{2B^2}$$

$$\sim \mathcal{O}(\epsilon_B^2)$$

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Guiding-center generating function

$$H = \frac{1}{2} m W_\parallel^2 + \frac{1}{2} m W_\perp^2 + m(W_\parallel \mathcal{W}_\parallel + W_\perp \mathcal{W}_\perp) + \mathcal{O}(\epsilon_B^2)$$

$$H_0 \qquad\qquad H_1 \sim \mathcal{O}(\epsilon_B)$$

- **Formal scales separation in the Poisson bracket**

$$\{F, G\}_{\rm gc} = \epsilon^{-1}\{F, G\}_{-1} + \{F, G\}_0 + \epsilon\{F, G\}_1$$

$$H_1 = \widetilde{H_1} + \langle H_1 \rangle \qquad\qquad \langle H_1 \rangle = (2\pi)^{-1} \int_0^{2\pi} {\rm d}\Theta \; H_1$$

$$\bar{H} = H_0 + \epsilon_B \left(\langle H_1 \rangle + \boxed{\widetilde{H_1} - \{S_1, H_0\}_{-1}} - \epsilon \{S_1, H_0\}_0 - \epsilon^2 \{S_1, H_0\}_1 \right) + \mathcal{O}(\epsilon_B^2)$$

$$\sim \mathcal{O}(\epsilon_B) \qquad \sim \mathcal{O}(\epsilon_B)$$

$$\boxed{\frac{\partial S_1}{\partial \Theta} + \epsilon \frac{m^2 c}{eB} (W_\parallel \widetilde{\mathcal{W}_\parallel} + W_\perp \widetilde{\mathcal{W}_\perp}) = 0}$$

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Guiding-center reduced dynamics

$$S_{\rm gc} = \epsilon^2 \frac{m^3 c^2}{e^2 B^2}\left[\frac{W_\perp^3}{3B}\hat{\perp}\cdot\nabla B + \frac{W_\parallel W_\perp^2}{8}\left((\hat{\boldsymbol\rho}\cdot\nabla)\hat{\mathbf b}\cdot\hat{\boldsymbol\rho} - (\hat{\perp}\cdot\nabla)\hat{\mathbf b}\cdot\hat{\perp}\right) + W_\parallel^2 W_\perp(\nabla\times\hat{\mathbf b})\cdot\hat{\boldsymbol\rho}\right]$$

$$S_1 \sim \mathcal{O}(\epsilon_B)$$

$$H = \frac{1}{2}mW_\parallel^2 + \frac{1}{2}mW_\perp^2 + m(W_\parallel\langle\mathcal{W}_\parallel\rangle + W_\perp\langle\mathcal{W}_\perp\rangle) = \frac{1}{2}mW_\parallel^2 + \mu B + \epsilon\frac{mc}{2e}W_\parallel\mu\hat{\mathbf b}\cdot(\nabla\times\hat{\mathbf b})$$

Moved to the symplectic part by a shift in $W_\parallel$

$$\gamma_{\rm gc} = \left[\frac{e}{\epsilon c}\mathbf{A}(\mathbf{X}) + mW_\parallel\hat{\mathbf b}(\mathbf{X}) - \epsilon\frac{mc}{e}\mu\mathbf{R}^*\right]\cdot \mathrm{d}\mathbf{X} + \epsilon\frac{mc}{e}\mu\mathrm{d}\Theta - H_{\rm gc}\mathrm{d}t + \mathcal{O}(\epsilon_B^2)$$

$$\nabla^* = \nabla - \mathbf{R}^*\frac{\partial}{\partial\theta}$$

$$H_{\rm gc} = \mu B(\mathbf{X}) + \frac{1}{2}mW_\parallel^2$$

$$\mathbf{B}^* = \mathbf{B} + \epsilon\frac{mc}{e}W_\parallel\nabla\times\hat{\mathbf b} - \epsilon^2\frac{mc^2}{e^2}\mu\nabla\times\mathbf{R}^*$$

$$\mathbf{R}^* = \nabla\hat{\mathbf b}_1\cdot\hat{\mathbf b}_2 + (\hat{\mathbf b}\cdot\nabla\times\hat{\mathbf b})\hat{\mathbf b}/2$$

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Guiding-center dynamical reduction

Homogeneous & Non-homogeneous magnetic field

Position and velocity shift
+
Gauge transformation:

Far from identity phase-space transformation

Larmor radius definition: **exact solution for SLAB** (homogeneous) magnetic field

Non-homogeneous magnetic field

Building a near-identity phase-space coordinate transformation via **gauge-transformations**

Goal: At the end of this step a symplectic part is free from gyroangle dependencies

↓

Poisson Bracket on the reduced phase space free from gyroangle dependencies **until the required order**

Non-homogeneous magnetic field

Final step:
Canonical Lie-transformation: on the Hamiltonian only (scalar function) use Poisson Bracket on the reduced phase space

Goal: remove all gyroangle dependencies from the Hamiltonian

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Gyrocenter dynamical reduction

- 1-form phase-space particle Lagrangian

$$\gamma_{\rm pert} \equiv L_{\rm pert} \cdot {\rm d}t = \left(\frac{e}{\epsilon c}\mathbf{A}(\mathbf{x}) + \epsilon_\delta \frac{e}{c}\mathbf{A}_1(\mathbf{x},t) + m\mathbf{v}\right) \cdot {\rm d}\mathbf{x} - H{\rm d}t,$$

$$H = \frac{1}{2}m\mathbf{v}^2 + \epsilon_\delta e\phi_1(\mathbf{x},t)$$

- Gyrocenter Velocity shift $\bar{\mathbf{v}} = \mathbf{v} + \epsilon_\delta \frac{e}{mc}\mathbf{A}_1(\mathbf{x},t)$

- Removes all the fluctuating fields from the symplectic part to the Hamiltonian part

$$\gamma_{\rm pert} = \left(\frac{e}{\epsilon c}\mathbf{A}(\mathbf{x}) + m\bar{\mathbf{v}}\right) \cdot {\rm d}\mathbf{x} - H{\rm d}t,$$

$$H = \frac{1}{2}m\bar{\mathbf{v}}^2 + \epsilon_\delta e\phi_1(\mathbf{x},t) - \epsilon_\delta \frac{e}{mc}\bar{\mathbf{v}} \cdot \mathbf{A}_1(\mathbf{x},t) + \epsilon_\delta^2 \left(\frac{e}{mc}\right)^2 \|\mathbf{A}_1(\mathbf{x},t)\|^2$$

- Starting reduction procedure from the “shiffted” particle phase-space $(\mathbf{x}, \bar{\mathbf{v}})$

Advantage: Only Canonical Lie- Transformations on the Hamiltonian part need to be performed. Significantly simplified derivation with respect to Brizard 1989.

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Recent achievements

- **Considering theory and numerical implementations simultaneously:**
  - **Theory***:*
    - Recovering existing code models from the variational GK framework
    - Comparing with model issued from the systematic theoretical derivation
    - *PIC ORB5 [**Tronko**, Bottino, Sonnendrücker, Phys. Plasmas 2016]*
    - *PIC ORB5; Eulerian GENE [**Tronko**, Bottino, Goerler et al, Phys.Plasmas 2017]*
    - *PIC ORB5 [**Tronko**, Bottino, Sonnendrücker, Chandre, PPCF, 2017]*
    - Verification of approximations consistency and regimes of applicability
    - Complete self-consistent GK rederivation from scratch with new clarified ordering
    - *[**Tronko** and Chandre, arXiv:1709.05222, 2017]*

  - **Intercode benchmark**: Implicit numerical schemes verification **[T.Goerler]**

    - **Microinstability characterization and investigation of required resolution**
    - Linear electromagnetic intercode benchmark (challenging)
    - *[**Görler**, Tronko, Hornsby, Bottino, Kleiber, Norscini, Grandgirard, Jenko and Sonnendrücker Phys.Plasmas. 2016]*
    - New electromagnetic physics
    - **Microturbulence investigation: extra –challenging work in progress**

$$\bar{\gamma}_{\rm pert} = \left(\frac{e}{\epsilon c}\mathbf{A}(\bar{\mathbf{X}}) + m\bar{v}_{\|}\hat{\mathbf{b}}(\bar{\mathbf{X}}) - \epsilon\frac{mc}{e}\mu\mathbf{R}^*\right)\cdot {\rm d}\bar{\mathbf{X}} + \epsilon\frac{mc}{e}\bar{\mu}{\rm d}\bar{\theta} - H{\rm d}t + \mathcal{O}(\epsilon_B^2)$$

$$\Gamma = \left(\frac{e}{\epsilon c}\mathbf{A}(\bar{\mathbf{X}}) + m\bar{v}_{\|}\hat{\mathbf{b}}(\bar{\mathbf{X}}) - \epsilon\frac{mc}{e}\mu\mathbf{R}^*\right)\cdot {\rm d}\bar{\mathbf{X}} + \epsilon\frac{mc}{e}\bar{\mu}{\rm d}\bar{\theta}$$

$$\{F,G\}_{\rm gc} = \frac{e}{\epsilon mc}\left(\frac{\partial F}{\partial\bar{\theta}}\frac{\partial G}{\partial\bar{\mu}} - \frac{\partial F}{\partial\bar{\mu}}\frac{\partial G}{\partial\bar{\theta}}\right) + \frac{\mathbf{B}^*}{mB_\|^*}\cdot\left(\nabla^* F\frac{\partial G}{\partial\bar{v}_\|} - \frac{\partial F}{\partial\bar{v}_\|}\nabla^* G\right) - \epsilon\frac{c\hat{\mathbf{b}}}{eB_\|^*}\cdot(\nabla^* F\times\nabla^* G)$$

$$\mathbf{R}^* = \nabla\hat{\mathbf{b}}_1\cdot\hat{\mathbf{b}}_2 + (\hat{\mathbf{b}}\cdot\nabla\times\hat{\mathbf{b}})\hat{\mathbf{b}}/2 \quad \sim\mathcal{O}(\epsilon_B)$$

$$\nabla^* = \nabla - \mathbf{R}^*\frac{\partial}{\partial\theta}$$

$$\mathbf{B}^* = \mathbf{B} + \epsilon\frac{mc}{e}\bar{v}_\|\nabla\times\hat{\mathbf{b}} - \epsilon^2\frac{mc^2}{e^2}\bar{\mu}\nabla\times\mathbf{R}^*$$

$$\sim\mathcal{O}(\epsilon_B^2)$$

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- Gauge-transformations
- Canonical Lie-transforms

How to build up a GK model consistently?

- All approximations **should** be performed on the Lagrangian L **before** deriving the equations of motion:
  - Approach guarantees energetic consistency of final equations
  - Symmetry properties of Lagrangian are automatically transferred to the equations
  - **Significant numerical advantage:** Use conserved quantities for building code diagnostics: ORB5 new physics of electromagnetic microinstabilities

- **Set up polarization effects into the system (choose from hierarchy of models):**
  - **Choice of the second order gyrocenter Hamiltonian defines reduced field- particles dynamics**

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- Formal scales separation in the Poisson bracket

$$\{F,G\}_{\rm gc} = \epsilon^{-1}\{F,G\}_{-1} + \{F,G\}_0 + \epsilon\{F,G\}_1$$

- Canonical Lie-transform

$$\bar{\mathcal{H}}(\mathbf{Z}) = \mathrm{e}^{-\pounds_S}\mathcal{H}(\mathbf{Z}) = \mathcal{H} - \{S,\mathcal{H}\} + \frac{1}{2}\{S,\{S,\mathcal{H}\}\} + \mathcal{O}(S^3)$$

- Guiding-center Poisson bracket on the extended phase space (to include time dependencies)

$$\{\mathcal{F},\mathcal{G}\} = \{\mathcal{F},\mathcal{G}\}_{\rm gc} + \frac{\partial\mathcal{F}}{\partial t}\frac{\partial\mathcal{G}}{\partial k} - \frac{\partial\mathcal{F}}{\partial k}\frac{\partial\mathcal{G}}{\partial t}$$

- Coordinate transform is constructed simultaneously $\quad \mathbf{Z} = \mathrm{e}^{\pounds_S}\mathbf{z}$

- Scalar invariance $\quad \bar{\mathcal{H}}(\mathbf{Z}) = \mathcal{H}(\mathbf{z})$

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- Generating function identification $S = \epsilon\epsilon_\delta S_1 + \epsilon\epsilon_\delta^2 S_2$
- Perturbative procedure: uses ordering on anisotropy of the turbulence

$$H_0 = \bar{\mu}B(\bar{\mathbf{X}}) + \frac{1}{2}m\bar{v}_\parallel^2, \qquad H_1 = e\psi_1(\bar{\mathbf{X}}, \bar{\theta}, \bar{\mu}, \bar{v}_\parallel, t), \qquad H_2 = \frac{e^2}{2mc^2}\|\mathbf{A}_1(\bar{\mathbf{X}} + \boldsymbol{\rho}, t)\|^2.$$

$$H_1 = \widetilde{H_1} + \langle H_1 \rangle \qquad \langle H_1 \rangle = (2\pi)^{-1}\int_0^{2\pi} \mathrm{d}\bar{\theta}\ H_1$$

$$\bar{\mathcal{H}} = k + H_0 + \epsilon_\delta \left(\langle H_1 \rangle + \widetilde{H_1} - \{S_1, H_0\}_{-1} - \epsilon\{S_1, H_0\}_0 - \epsilon^2\{S_1, H_0\}_1 - \epsilon\frac{\partial S_1}{\partial t}\right) + \mathcal{O}(\epsilon_\delta^2).$$

$$\sim \mathcal{O}(\epsilon_\parallel) \qquad \sim \mathcal{O}(\epsilon_B) \qquad \sim \mathcal{O}(\epsilon_\omega)$$

$$\{S_1, H_0\}_{-1} = \frac{eB}{mc}\frac{\partial S_1}{\partial \bar{\theta}} = \widetilde{H_1}$$

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Gyrocenter change of coordinate

- Gyrocenter change of coordinates

$$\mathbf{x} = \bar{\mathbf{X}} + \epsilon \frac{mc}{eB}\hat{\mathbf{b}} \times \bar{\mathbf{v}} = \bar{\mathbf{X}} + \epsilon \frac{mc}{eB}\hat{\mathbf{b}} \times \mathbf{v} + \epsilon\epsilon_\delta \frac{1}{B}\hat{\mathbf{b}} \times \mathbf{A}_1 + \mathcal{O}(\epsilon_\delta^2).$$

$$\mathbf{x} = \bar{\mathbf{X}} + \boxed{\epsilon \boldsymbol{\rho}_0} + \boxed{\epsilon_\delta \boldsymbol{\rho}_1}$$

Guiding-center displacement

$$\boldsymbol{\rho}_1 = -\left\{ S_1, \left(\bar{\mathbf{X}} + \epsilon\boldsymbol{\rho}_0 + \epsilon\epsilon_\delta \frac{1}{B}\hat{\mathbf{b}} \times \mathbf{A}_1 \right) \right\}_{-1}$$

Gyrocenter displacement

$$\boldsymbol{\rho} = \boldsymbol{\rho}_0 + \epsilon\epsilon_\delta \frac{1}{B}\hat{\mathbf{b}} \times \mathbf{A}_1(\bar{\mathbf{X}} + \boldsymbol{\rho}_0, t),$$

Shiffted guiding-center displacement

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$$H_{\rm gy} = H_{\rm gc} + \epsilon_\delta e\langle\Psi_1\rangle + \epsilon_\delta^2 e^2\left(\frac{1}{2mc^2}\langle\|\mathbf{A}_1\|^2\rangle - \frac{1}{2B}\frac{\partial}{\partial\mu_{\rm gy}}(\langle\Psi_1^2\rangle - \langle\Psi_1\rangle^2)\right)$$

$$+\,\epsilon_\delta^2\left(\epsilon\frac{e}{B}\langle\hat{\mathbf{b}}\times\mathbf{A}_1\cdot\nabla\Psi_1\rangle - \epsilon^2\frac{mc^2}{2B^2}\hat{\mathbf{b}}\cdot\left\langle\nabla\widetilde{\Psi_1}\times\int \mathrm{d}\theta_{\rm gy}\nabla\widetilde{\Psi_1}\right\rangle\right),$$

$$\Psi_1(\mathbf{X}_{\rm gy},\theta_{\rm gy},\mu_{\rm gy},v_{\|\rm gy},t) = \phi_1(\mathbf{X}_{\rm gy}+\boldsymbol{\rho}_0,t) - \frac{v_{\|\rm gy}}{c}\hat{\mathbf{b}}(\mathbf{X}_{\rm gy})\cdot\mathbf{A}_1(\mathbf{X}_{\rm gy}+\boldsymbol{\rho}_0,t)$$

$$-\sqrt{\frac{2\mu_{\rm gy}B(\mathbf{X}_{\rm gy})}{mc^2}}\,\hat{\perp}(\theta_{\rm gy},\mathbf{X}_{\rm gy})\cdot\mathbf{A}_1(\mathbf{X}_{\rm gy}+\boldsymbol{\rho}_0,t)$$