Metriplectic dynamics:

A framework for kinetic theory and numerics

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Motivation: EXASCALE COMPUTING

- **EXASCALE IS COMING:** The near-future increase in computational resources is expected to enable kinetic simulations of plasmas that extend to macroscopic, even thermodynamic time scales.
- **PHYSICS IS SYMMETRY AND CONSERVATION LAWS:** Existing simulation methods for dissipative systems are largely based on instantaneous error estimation and typically fail in achieving long-time-scale stability and accuracy.
- **MATHEMATICS COULD HELP:** The recent interest towards and development of structure-preserving techniques reflects the future of kinetic simulation algorithms for plasmas and could be the game changer.

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The metriplectic framework

Metriplectic framework describes dynamics of functionals

The dynamics of a functional Q of fields $u = (u^1, \ldots, u^m)$ is determined in terms of a Hamiltonian H, a Poisson bracket $\{\cdot, \cdot\}$, an entropy functional S, and a metric bracket $(\cdot, \cdot)$ according to

$$\frac{dQ}{dt} = \{Q, F\} + (Q, F),$$

where $F = H - S$ is a generalized free-energy functional akin to the Gibb's free energy [1].

The First and Second Laws of Thermodynamics are satisfied

Impose (i) $(H, A) = 0$ and (ii) $\{S, A\} = 0$ for arbitrary A as well as (iii) $(A, A) \leq 0$. Then (i) and (ii) imply the conservation of the Hamiltonian

$$\frac{dH}{dt} = \{H, F\} + (H, F) = -\{H, S\} + (H, F) = 0,$$

the condition (iii) implies the dissipation of the free energy

$$\frac{dF}{dt} = \{F, F\} + (F, F) = (F, F) \leq 0,$$

and the conditions (i), (ii), and (iii) all together imply the production of entropy

$$\frac{dS}{dt} = \{S, F\} + (S, F) = (S, H - S) = -(S, S) \geq 0.$$

The brackets are bilinear functionals

The generic forms for the brackets involve an anti-self-adjoint operator $J(u)$, a self-adjoint operator $G(u)$, and functional derivatives

$$\{A, B\} = \int \frac{\delta A}{\delta u^\alpha} J^{\alpha\beta}(u) \frac{\delta B}{\delta u^\beta} dx,$$
$$(A, B) = \int \frac{\delta A}{\delta u^\alpha} G^{\alpha\beta}(u) \frac{\delta B}{\delta u^j} dx.$$

The functional derivative $\delta A/\delta u^\alpha$ is defined via the Fréchet derivative

$$\frac{d}{d\epsilon} A[u^1, \ldots, u^\alpha + \epsilon v^\alpha, \ldots, u^m]\big|_{\epsilon=0} = \left\langle \frac{\delta A[u]}{\delta u^\alpha}, v^\alpha \right\rangle,$$

with $\langle \cdot\,, \cdot \rangle$ denoting an appropriate inner product. Note that the functional derivative $\delta A/\delta u^\alpha$ is an element of the dual space, while the field u^α is an element of the primal space. This has consequences for discretization.

Existence of an equilibrium state

Remember that the dynamics is given by

$$\frac{dQ}{dt} = \{Q, F\} + (Q, F),$$

For an equilibrium state u_{eq} to exists, time-evolution of all functionals must vanish when evaluated with respect to u_{eq}. This leads to so-called Energy-Casimir principle

$$\delta F[u_{\mathsf{eq}}] + \sum_i \lambda_i \delta C_i[u_{\mathsf{eq}}] = 0,$$

where C_i are Casimirs ($\{C_i, A\} + (C_i, A) = 0$ for arbitrary A) of the total metriplectic system and λ_i act as Lagrange multipliers that are uniquely determined from the initial state of the system.

Metriplectic formulation of collisional kinetic theory

Vlasov-Maxwell-Landau system

The dynamic equations push the distribution functions and the electromagnetic fields

$$\begin{aligned}
\frac{\partial f_s}{\partial t} &= -\boldsymbol{v}\cdot\nabla f_s - \frac{e_s}{m_s}(\boldsymbol{E}+\boldsymbol{v}\times\boldsymbol{B})\cdot\frac{\partial f_s}{\partial \boldsymbol{v}} + C[f_s],\\
\frac{1}{c^2}\frac{\partial \boldsymbol{E}}{\partial t} &= \nabla\times\boldsymbol{B} - \mu_0\sum_s e_s\int \boldsymbol{v} f_s\, d\boldsymbol{v},\\
\frac{\partial \boldsymbol{B}}{\partial t} &= -\nabla\times\boldsymbol{E},
\end{aligned}$$

The static, constraining equations serve as initial conditions

$$\varepsilon_0\nabla\cdot\boldsymbol{E} = \sum_s e_s\int f_s\, d\boldsymbol{v}, \qquad \nabla\cdot\boldsymbol{B} = 0$$

The collision operator $C[f_s]$, provides dissipation

$$C[f_s] = \sum_{s'}\frac{c_{ss'}}{m_s}\frac{\partial}{\partial \boldsymbol{v}}\cdot\int \mathbb{Q}(\boldsymbol{v}-\boldsymbol{v}')\cdot\left(\frac{f_{s'}(\boldsymbol{v}')}{m_s}\frac{\partial f_s}{\partial \boldsymbol{v}} - \frac{f_s(\boldsymbol{v})}{m_{s'}}\frac{\partial f_{s'}}{\partial \boldsymbol{v'}}\right) d\boldsymbol{v}'$$

with $\mathbb{Q}(\boldsymbol{\xi}) = |\boldsymbol{\xi}|^{-1}(\mathbf{1}-\hat{\boldsymbol{\xi}}\hat{\boldsymbol{\xi}})$ and $c_{ss'} = e_s^2 e_{s'}^2 \ln\Lambda/(8\pi\varepsilon_0^2)$.

Hamiltonian contribution

Poisson bracket consists of single-particle, interaction, and electromagnetic contributions

$$\begin{aligned}\{\mathcal{A},\mathcal{B}\} = &\sum_s \int f_s \left[\frac{\delta \mathcal{A}}{\delta f_s}, \frac{\delta \mathcal{B}}{\delta f_s}\right]_s d\boldsymbol{x}d\boldsymbol{v} \\ &+ \sum_s \int \frac{e_s f_s}{\varepsilon_0 m_s} \left(\frac{\partial}{\partial \boldsymbol{v}} \frac{\delta \mathcal{A}}{\delta f_s} \cdot \frac{\delta \mathcal{B}}{\delta \boldsymbol{E}} - \frac{\partial}{\partial \boldsymbol{v}} \frac{\delta \mathcal{B}}{\delta f_s} \cdot \frac{\delta \mathcal{A}}{\delta \boldsymbol{E}}\right) d\boldsymbol{x}d\boldsymbol{v} \\ &+ \epsilon_0^{-1} \int \left(\nabla \times \frac{\delta \mathcal{A}}{\delta \boldsymbol{E}} \cdot \frac{\delta \mathcal{B}}{\delta \boldsymbol{B}} - \nabla \times \frac{\delta \mathcal{B}}{\delta \boldsymbol{E}} \cdot \frac{\delta fa}{\delta \boldsymbol{B}}\right) d\boldsymbol{x}\end{aligned}$$

Hamiltonian is a sum of kinetic and electromagnetic energy

$$\mathcal{H}[f, \boldsymbol{E}, \boldsymbol{B}] = \sum_s \int \frac{m_s v^2}{2} f_s d\boldsymbol{x}d\boldsymbol{v} + \frac{1}{2} \int \left(\epsilon_0 \boldsymbol{E}^2 + \mu_0^{-1} \boldsymbol{B}^2\right) d\boldsymbol{x}$$

Single-particle non-canonical Poisson bracket for species s

$$[f, g]_s = \frac{1}{m_s} \left(\nabla f \cdot \frac{\partial g}{\partial \boldsymbol{v}} - \nabla g \cdot \frac{\partial f}{\partial \boldsymbol{v}}\right) + \frac{e_s \boldsymbol{B}}{m_s^2} \cdot \frac{\partial f}{\partial \boldsymbol{v}} \times \frac{\partial g}{\partial \boldsymbol{v}}$$

Dissipative contribution

The bracket corresponding to Landau collision operator [1, 2]

$$(\mathcal{A}, \mathcal{B}) = \sum_{s,s'} \int \int \boldsymbol{\Gamma}_{ss'}(\mathcal{A}; \boldsymbol{z}, \boldsymbol{z}') \cdot \mathbb{W}_{ss'}(\boldsymbol{z}, \boldsymbol{z}') \cdot \boldsymbol{\Gamma}_{ss'}(\mathcal{B}; \boldsymbol{z}, \boldsymbol{z}') d\boldsymbol{z} d\boldsymbol{z}'$$

Entropy functional corresponding to Maxwell-Boltzmann statistics

$$\mathcal{S}[f] = -\sum_{s} \int f_s(\boldsymbol{z}) \ln \left(f_s(\boldsymbol{z}) \right) d\boldsymbol{z}$$

Details for vector $\boldsymbol{\Gamma}$ and matrix $\mathbb{W}$ in the bracket

$$\boldsymbol{\Gamma}_{ss'}(\mathcal{A}; \boldsymbol{z}, \boldsymbol{z}') = \frac{1}{m_s} \frac{\partial}{\partial \boldsymbol{v}} \frac{\delta \mathcal{A}}{\delta f_s(\boldsymbol{z})} - \frac{1}{m_{s'}} \frac{\partial}{\partial \boldsymbol{v}'} \frac{\delta \mathcal{A}}{\delta f_{s'}(\boldsymbol{z}')}$$

$$\mathbb{W}_{ss'}(\boldsymbol{z}, \boldsymbol{z}') = -\tfrac{1}{2} c_{ss'} \delta(\boldsymbol{x} - \boldsymbol{x}') f_s(\boldsymbol{z}) f_{s'}(\boldsymbol{z}') \mathbb{Q}(\boldsymbol{v} - \boldsymbol{v}')$$

again with $\mathbb{Q}(\boldsymbol{\xi}) = |\boldsymbol{\xi}|^{-1}(\mathbf{1} - \hat{\boldsymbol{\xi}}\hat{\boldsymbol{\xi}})$ and $c_{ss'} = e_s^2 e_{s'}^2 \ln \Lambda / (8\pi\varepsilon_0^2)$.

Invariants of the Vlasov-Maxwell-Landau system

The Gauss's laws: for arbitrary functions $g_E(\boldsymbol{x})$ and $g_B(\boldsymbol{x})$, one finds the Casimir invariants

$$\mathcal{C}_E = \int g_E(\boldsymbol{x}) \left(\varepsilon_0 \nabla \cdot \boldsymbol{E} - \sum_s e_s \int f_s \, d\boldsymbol{v} \right) d\boldsymbol{x}$$

$$\mathcal{C}_B = \int g_B(\boldsymbol{x}) \nabla \cdot \boldsymbol{B} d\boldsymbol{x}$$

If $\mathcal{C}_E$ and $\mathcal{C}_B$ are zero initially, they will remain so later on. The total momentum functional

$$\mathcal{P} = \sum_s m_s \int \boldsymbol{v} f_s d\boldsymbol{z} + \varepsilon_0 \int \boldsymbol{E} \times \boldsymbol{B} d\boldsymbol{x}$$

is conserved if the Gauss's law for $\boldsymbol{E}$ holds. The total energy, the Hamiltonian $\mathcal{H}$ is conserved by construction. Also mass of each species is conserved.

Metriplectic integrator for the Landau collision operator

Single species Landau operator

The collisional evolution of a distribution function in velocity space is given by the nonlinear Fokker-Planck equation

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial v} \cdot \int Q(v - v') \cdot \left(f(v') \frac{\partial f}{\partial v} - f(v) \frac{\partial f}{\partial v'} \right) dv' \tag{1}$$

With entropy $S[f] = -\int f \ln(f) dv$, the corresponding bracket is

$$(\mathcal{A}, \mathcal{B}) = -\frac{1}{2} \int \int \Gamma(\mathcal{A}; v, v') \cdot W(v, v') \cdot \Gamma(\mathcal{B}; v, v') dv dv' \tag{2}$$

with the vector Γ and the tensor W defined as

$$\Gamma(\mathcal{A}; v, v') = \left(\frac{\partial}{\partial v} \frac{\delta \mathcal{A}}{\delta f(v)} - \frac{\partial}{\partial v'} \frac{\delta \mathcal{A}}{\delta f(v')} \right) \tag{3}$$

$$W(v, v') = f(v) f(v') Q(v - v'). \tag{4}$$

The bracket has three Casimirs $\{\mathcal{M}, \mathcal{P}, \mathcal{E}\} = \int \{1, v, |v|^2\} f dv$, i.e., mass and kinetic momentum and energy. The first two follow from $\Gamma(\mathcal{M}) = 0$ and $\Gamma(\mathcal{P}) = 0$, and the last from $\Gamma(\mathcal{E}) = 2(v - v')$ and $\xi \cdot Q(\xi) = 0$.

Discretize the system with finite-elements

We consider a finite-dimensional space $Q_h(\Omega) \subset L^2(\Omega)$ spanned by a set of basis functions $\{\phi_i\}_{i=1}^N$ and write the discrete distribution function $f_h \in Q_h(\Omega)$ in this space as

$$f_h = \sum_{i=1}^{N} \hat{f}_i(t)\phi_i(v). \tag{5}$$

Functionals $\mathcal{A}$ evaluated with respect to f_h become functions $\mathcal{A}[f_h] = \widehat{A}(\hat{f})$ of the degrees of freedom $\hat{f} = (\hat{f}_1, \ldots, \hat{f}_N)$.

Functional derivatives evaluated with respect to f_h become

$$\frac{\delta \mathcal{A}[f_h]}{\delta f} = \sum_{i,j=1}^{N} \frac{\partial \widehat{A}}{\partial \hat{f}_i} \mathbb{M}_{ij}^{-1} \phi_j, \tag{6}$$

where $\mathbb{M}_{ij} = \int \phi_i(v)\phi_j(v)dv$ is the mass matrix for the basis ϕ_j.

Obtaining the discrete bracket

Insert the expressions for f_h and $\delta\mathcal{A}[f_h]/\delta f$ into the continuous bracket to obtain

$$(\mathcal{A},\mathcal{B})[f_h] = \nabla\widehat{A}\,\mathbb{M}^{-1}\,\mathbb{L}\,\mathbb{M}^{-1}\,\nabla\widehat{B} \equiv \nabla\widehat{A}\,\mathbb{G}\,\nabla\widehat{B} \equiv (\widehat{A},\widehat{B})_h. \tag{7}$$

The gradient refers to $\nabla = \partial/\partial\hat{f}$ and the elements of the Landau matrix $\mathbb{L}$ are given by

$$\mathbb{L}_{ij}(\hat{f}) = -\frac{1}{2}\int\int\left(\frac{\partial\phi_i}{\partial v} - \frac{\partial\phi_i}{\partial v'}\right) \cdot f_h(v)Q(v-v')f_h(v')\cdot\left(\frac{\partial\phi_j}{\partial v} - \frac{\partial\phi_j}{\partial v'}\right)dvdv' \tag{8}$$

Choose a space of at least second order polynomials

Choose the space $Q_h(\Omega)$ so that $\{1, v, |v|^2\} \in Q_h(\Omega)$. Now the mass, momentum, and energy functionals evaluated with respect to f_h become

$$\mathcal{M}[f_h] = \sum_{i=1}^{N} \hat{f}_i \int \phi_i dv = \hat{1}\mathbb{M}\hat{f} \equiv \widehat{M}(\hat{f}) \tag{9}$$

$$\mathcal{P}[f_h] = \sum_{i=1}^{N} \hat{f}_i \int v\phi_i dv = \hat{v}\mathbb{M}\hat{f} \equiv \widehat{P}(\hat{f}) \tag{10}$$

$$\mathcal{E}[f_h] = \sum_{i=1}^{N} \hat{f}_i \int |v|^2\phi_i dv = \hat{e}\mathbb{M}\hat{f} \equiv \widehat{E}(\hat{f}) \tag{11}$$

with $\hat{1}$, $\hat{v}$, and $\hat{e}$ the degrees of freedom for the functions 1, v, and $|v|^2$. Note that $\widehat{M}(\hat{f})$, $\widehat{P}(\hat{f})$, and $\widehat{E}(\hat{f})$ are linear functions of $\hat{f}$.

Casimir invariants of the discrete Landau bracket

The Landau matrix $\mathbb{L}(\hat{f})$ has the important properties

$$\hat{1}\,\mathbb{L} = 0, \quad \hat{v}\,\mathbb{L} = 0, \quad \hat{e}\,\mathbb{L} = 0 \tag{12}$$

This implies that the quantities $\widehat{M}(\hat{f})$, $\widehat{P}(\hat{f})$, and $\widehat{E}(\hat{f})$ are Casimirs:

$$(\widehat{M}, \widehat{B})_h = \nabla \widehat{M}\,\mathbb{G}\,\nabla \widehat{B} = \hat{1}\mathbb{M}\mathbb{M}^{-1}\mathbb{L}\mathbb{M}^{-1}\nabla \widehat{B} = \hat{1}\mathbb{L}\mathbb{M}^{-1}\nabla \widehat{B} = 0 \tag{13}$$

$$(\widehat{P}, \widehat{B})_h = \nabla \widehat{P}\,\mathbb{G}\,\nabla \widehat{B} = \hat{v}\mathbb{M}\mathbb{M}^{-1}\mathbb{L}\mathbb{M}^{-1}\nabla \widehat{B} = \hat{v}\mathbb{L}\mathbb{M}^{-1}\nabla \widehat{B} = 0 \tag{14}$$

$$(\widehat{E}, \widehat{B})_h = \nabla \widehat{E}\,\mathbb{G}\,\nabla \widehat{B} = \hat{1}\mathbb{M}\mathbb{M}^{-1}\mathbb{L}\mathbb{M}^{-1}\nabla \widehat{B} = \hat{e}\mathbb{L}\mathbb{M}^{-1}\nabla \widehat{B} = 0 \tag{15}$$

Since $\widehat{M}(\hat{f})$, $\widehat{P}(\hat{f})$, and $\widehat{E}(\hat{f})$ are linear functionals, they are linear Casimirs.

Temporal integration with "Discrete Gradients"

In terms of free energy $\widehat{F}(\hat{f}) = \widehat{E}(\hat{f}) - \widehat{S}(\hat{f})$, the equations of motion for the degrees of freedom are

$$\frac{d\hat{f}}{dt} = (\hat{f}, \widehat{F})_h = \mathbb{G}\,\nabla\widehat{F}$$

We use a so-called "discrete gradient" $\bar{\nabla}$ of a differentiable function $h : \mathbb{R}^m \to \mathbb{R}$ with the property

$$\begin{aligned}(x_1 - x_0) \cdot \bar{\nabla} h(x_0, x_1) = h(x_1) - h(x_0),\\ \bar{\nabla} h(x, x) = \nabla h(x).\end{aligned} \tag{16}$$

and introduce temporal discretization according to

$$\frac{\hat{f}_1 - \hat{f}_0}{\Delta t} = \mathbb{G}(\hat{f}_{1/2})\,\bar{\nabla}\widehat{F}(\hat{f}_0, \hat{f}_1), \tag{17}$$

where $\hat{f}_{1/2} = (\hat{f}_0 + \hat{f}_1)/2$.

Dissipation of free-energy, production of entropy, and preservation of the Casimir invariants

The negative-semidefiniteness of $\mathbb{G}$ implies dissipation of free energy

$$\frac{\widehat{F}(\hat{f}_1) - \widehat{F}(\hat{f}_0)}{\Delta t} = \bar{\nabla}\widehat{F}(\hat{f}_0, \hat{f}_1)\,\mathbb{G}(\hat{f}_{1/2})\,\bar{\nabla}\widehat{F}(\hat{f}_0, \hat{f}_1) \leq 0 \tag{18}$$

The linear Casimirs $\widehat{C} \in \{\widehat{M}(\hat{f}), \widehat{P}(\hat{f}), \widehat{E}(\hat{f})\}$ satisfy $\nabla\widehat{C}\mathbb{G} = 0$, and $(\hat{f}_1 - \hat{f}_0) \cdot \nabla\widehat{C} = \widehat{C}(\hat{f}_1) - \widehat{C}(\hat{f}_0)$, and are thus preserved

$$\frac{\widehat{C}(\hat{f}_1) - \widehat{C}(\hat{f}_0)}{\Delta t} = \nabla\widehat{C}\,\mathbb{G}(\hat{f}_{1/2})\,\bar{\nabla}\widehat{F}(\hat{f}_0, \hat{f}_1) = 0 \tag{19}$$

Entropy production is guaranteed via dissipation of the free energy $\widehat{F}$ and preservation of $\widehat{E}$ via

$$\widehat{S}_1 - \widehat{S}_0 = \widehat{E}_1 - \widehat{F}_1 - \widehat{E}_0 + \widehat{F}_0 = \widehat{F}_0 - \widehat{F}_1 \geq 0.$$

Summary

Kinetic descriptions of plasmas appear to be metriplectic

- **The Vlasov-Maxwell-Landau system** is metriplectic.
- **The collisional electrostatic gyrokinetic Vlasov-Poisson-Landau system** is metriplectic.
- Most likely **the collisional electromagnetic gyrokinetic Vlasov-Maxwell-Landau system** is metriplectic as well. This is work in progress.

Can we find metriplectic discretization techniques for the Vlasov-Maxwell-Landau system and its gyrokinetic versions?

	Particle-in-Cell	Grid Based
Poisson Integrators	GEMPIC	?
Metriplectic Integrators	?	Current Work

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Metriplectic formulation of collisional electrostatic gyrokinetics

Collisional electrostatic gyrokinetic equations [3]

Dynamic kinetic equation and static Gauss' law

$$\frac{\partial F_s}{\partial t} + \{F_s, H_s^{\mathsf{gy}}\}_s^{\mathsf{gc}} = \sum_{\bar{s}} C_{s\bar{s}}^{\mathsf{gy}}(F_s, F_{\bar{s}}), \tag{20}$$

$$\nabla \cdot \boldsymbol{E} = 4\pi(\rho_{\mathsf{gy}} - \nabla \cdot \boldsymbol{P}), \tag{21}$$

Guiding-center Poisson bracket

$$\begin{aligned}\{F, G\}^{\mathsf{gc}} =& \frac{e}{mc}\left(\frac{\partial F}{\partial \theta}\frac{\partial G}{\partial \mu} - \frac{\partial F}{\partial \mu}\frac{\partial G}{\partial \theta}\right) - \frac{c\boldsymbol{b}}{eB_\parallel^*} \cdot (\nabla^* F \times \nabla^* G) \\ &+ \frac{\boldsymbol{B}^*}{mB_\parallel^*} \cdot \left(\nabla^* F \frac{\partial G}{\partial v_\parallel} - \frac{\partial F}{\partial v_\parallel}\nabla^* G\right),\end{aligned} \tag{22}$$

Gyrocenter Hamiltonian $H^{\mathsf{gy}} = K^{\mathsf{gy}} + e\varphi$, and polarization density

$$\boldsymbol{P} = -\delta\mathcal{K}/\delta\boldsymbol{E}, \qquad \mathcal{K}(\boldsymbol{E}) = \sum_s \int K_s^{\mathsf{gy}}\, F_s\, d\boldsymbol{z}_s^{\mathsf{gc}}, \tag{23}$$

Gyrocenter kinetic energy K^{gy} contains the nasty details

The function K^{gy}, appearing in the Hamiltonian $H^{\mathrm{gy}} = K^{\mathrm{gy}} + e\varphi$, is the gyrocenter kinetic energy, which may be written entirely in terms of the electric field as

$$\begin{aligned} K^{\mathrm{gy}} =& \frac{1}{2} m v_\parallel^2 + \mu |\boldsymbol{B}| - e \langle [\![\boldsymbol{\rho}_o \cdot \boldsymbol{E}(\boldsymbol{X} + \epsilon \boldsymbol{\rho}_o)]\!] \rangle \\ & - \frac{e^2}{2\mu|\boldsymbol{B}|} \langle [\![\widetilde{\boldsymbol{\rho}_o \cdot \boldsymbol{E}}(\boldsymbol{X} + \epsilon\boldsymbol{\rho}_o) \widetilde{\boldsymbol{\rho}_o \cdot \boldsymbol{E}}(\boldsymbol{X} + \boldsymbol{\rho}_o)]\!] \rangle \\ & - \frac{e^2}{2m\omega_c^2} \boldsymbol{b} \cdot \langle \tilde{\boldsymbol{E}}(\boldsymbol{X} + \boldsymbol{\rho}_o) \times I \tilde{\boldsymbol{E}}(\boldsymbol{X} + \boldsymbol{\rho}_o) \rangle. \end{aligned} \quad (24)$$

Here $\langle \cdot \rangle_s = (2\pi)^{-1} \int_0^{2\pi} \cdot \, d\theta_s$ denotes the average with respect to the species-s gyroangle, tildes denote the fluctuating part of a gyroangle-dependent quantity, $I = \partial_\theta^{-1}$ is the gyroangle antiderivative, $[\![\cdot]\!] = \int_0^1 \cdot \, d\epsilon$, and $\boldsymbol{\rho}_o$ is the zero'th order (gyroangle-dependent) gyroradius vector.

The electrostatic gyrocenter collision operator $C^{\mathsf{gy}}_{s\bar{s}}(F_s, F_{\bar{s}})$

Define the position $\boldsymbol{y}_s(\boldsymbol{z}) = \boldsymbol{X} + \boldsymbol{\rho}_{os}$, the relative velocity

$$\boldsymbol{w}^{\mathsf{gy}}_{s\bar{s}} = \{\boldsymbol{y}_s, H^{\mathsf{gy}}_s\}^{\mathsf{gc}}_s(\boldsymbol{z}) - \{\boldsymbol{y}_{\bar{s}}, H^{\mathsf{gy}}_s\}^{\mathsf{gc}}_{\bar{s}}(\bar{\boldsymbol{z}}), \tag{25}$$

the scaled projection matrix

$$\mathbb{Q}^{\mathsf{gy}}_{s\bar{s}}(\boldsymbol{z}, \bar{\boldsymbol{z}}) = \frac{\mathbb{P}(\boldsymbol{w}^{\mathsf{gy}}_{s\bar{s}}(\boldsymbol{z}, \bar{\boldsymbol{z}}))}{w^{\mathsf{gy}}_{s\bar{s}}(\boldsymbol{z}, \bar{\boldsymbol{z}})}, \qquad \mathbb{P}(\boldsymbol{\xi}) = \mathbb{I} - \frac{\boldsymbol{\xi}\boldsymbol{\xi}}{|\boldsymbol{\xi}|^2}, \tag{26}$$

and the three-component collisional flux vector

$$\boldsymbol{\gamma}^{\mathsf{gy}}_{s\bar{s}} = \int \delta^{\mathsf{gy}}_{s\bar{s}}(\boldsymbol{z}, \bar{\boldsymbol{z}}) \mathbb{Q}^{\mathsf{gy}}_{s\bar{s}}(\boldsymbol{z}, \bar{\boldsymbol{z}}) \cdot \boldsymbol{A}^{\mathsf{gy}}_{s\bar{s}}(\boldsymbol{z}, \bar{\boldsymbol{z}})\, d\bar{\boldsymbol{z}}^{\mathsf{gc}}_{\bar{s}}, \tag{27}$$

where $\boldsymbol{A}^{\mathsf{gy}}_{s\bar{s}}(\boldsymbol{z}, \bar{\boldsymbol{z}}) = F_s(\boldsymbol{z})\{\bar{\boldsymbol{y}}_{\bar{s}}, F_{\bar{s}}(\bar{\boldsymbol{z}})\}^{\mathsf{gc}}_{\bar{s}} - F_{\bar{s}}(\bar{z})\{\boldsymbol{y}_s, F_s(\boldsymbol{z})\}^{\mathsf{gc}}_s$, and $\delta^{\mathsf{gy}}_{s\bar{s}}(\boldsymbol{z}, \bar{\boldsymbol{z}}) = \delta(\boldsymbol{y}_s - \bar{\boldsymbol{y}}_{\bar{s}})$. Defining the coefficient $c_{s\bar{s}} = 4\pi e_s^2 e_{\bar{s}}^2 \ln\Lambda$, the collision operator can then be expressed as

$$C^{\mathsf{gy}}_{s\bar{s}}(F_s, F_{\bar{s}}) = -\frac{c_{s\bar{s}}}{2} \left\langle \{y_{s,i}, \gamma^{\mathsf{gy}}_{s\bar{s},i}\}^{\mathsf{gc}}_s \right\rangle_s . \tag{28}$$

Metriplectic structure of collisional electrostatic gyrokinetics

Hamiltonian functional

$$\mathcal{H}_{\mathsf{GK}} = \sum_s \int H_s^{\mathsf{gy}} F_s \, d\boldsymbol{z}_s^{\mathsf{gc}} - \frac{1}{8\pi} \int |\boldsymbol{E}|^2 \, d^3\boldsymbol{x} \tag{29}$$

Entropy functional

$$\mathcal{S}_{\mathrm{GK}} = -\sum_s \int F_s(\boldsymbol{z}) \ln F_s(\boldsymbol{z}) d\boldsymbol{z}_s^{\mathsf{gc}}. \tag{30}$$

Metriplectic dynamics of arbitrary functionals $\mathcal{Q}[F]$ are given by

$$\frac{d\mathcal{Q}}{dt} = \{\mathcal{Q}, \mathcal{F}_{\mathsf{GK}}\}_{\mathsf{GK}} + (\mathcal{Q}, \mathcal{F}_{\mathsf{GK}})_{\mathsf{GK}}, \tag{31}$$

where $\mathcal{F}_{\mathsf{GK}} = \mathcal{H}_{\mathsf{GK}} - \mathcal{S}_{\mathsf{GK}}$ denotes the generalized free-energy functional that is dissipated via increase in the system entropy.

Hamiltonian contribution

The dynamical field in this system is F. The electrostatic potential must be regarded as the unique functional of the distribution function given by solving the gyrokinetic Poisson equation, i.e. $\varphi = \varphi[F]$.

The expression for the functional Poisson bracket of two functionals $\mathcal{A}(F)$ and $\mathcal{B}(F)$ is then given by

$$\{\mathcal{A}, \mathcal{B}\}_{\mathsf{GK}} = \sum_s \int \left\{ \frac{\delta \mathcal{A}}{\delta F_s}, \frac{\delta \mathcal{B}}{\delta F_s} \right\}_s^{\mathsf{gc}} F_s \, d\boldsymbol{z}_s^{\mathsf{gc}}, \tag{32}$$

Metric contribution

The symmetric bracket corresponding to the collision operator [4]

$$(\mathcal{A}, \mathcal{B})_{\mathrm{GK}} = -\sum_{s\bar{s}} \frac{c_{s\bar{s}}}{4} \iint \boldsymbol{\Gamma}^{\mathsf{gy}}_{s\bar{s}}(\mathcal{A}) \cdot \mathbb{W}^{\mathsf{gy}}_{s\bar{s}} \cdot \boldsymbol{\Gamma}^{\mathsf{gy}}_{s\bar{s}}(\mathcal{B}) d\boldsymbol{z}^{\mathsf{gc}}_{\bar{s}} d\boldsymbol{z}^{\mathsf{gc}}_{s}, \tag{33}$$

The vector $\boldsymbol{\Gamma}^{\mathsf{gy}}_{s\bar{s}}(\mathcal{A})$ is defined

$$\boldsymbol{\Gamma}^{\mathsf{gy}}_{s\bar{s}}(\mathcal{A}) = \left\{ \boldsymbol{y}_{\bar{s}}, \frac{\delta \mathcal{A}}{\delta F_{\bar{s}}} \right\}^{\mathsf{gc}}_{\bar{s}} (\bar{\boldsymbol{z}}) - \left\{ \boldsymbol{y}_{s}, \frac{\delta \mathcal{A}}{\delta F_{s}} \right\}^{\mathsf{gc}}_{s} (\boldsymbol{z}), \tag{34}$$

and the symmetric, positive semi-definite tensor $\mathbb{W}^{\mathsf{gy}}_{s\bar{s}}$ is

$$\mathbb{W}^{\mathsf{gy}}_{s\bar{s}} = \delta^{\mathsf{gy}}_{s\bar{s}}(\boldsymbol{z}, \bar{\boldsymbol{z}}) \mathbb{Q}_{s\bar{s}}(\boldsymbol{z}, \bar{\boldsymbol{z}}) F_s(\boldsymbol{z}) F_{\bar{s}}(\bar{\boldsymbol{z}}), \tag{35}$$

with $\delta^{\mathsf{gy}}_{s\bar{s}}$ and $\mathbb{Q}_{s\bar{s}}$ as before.

Energy conservation law

Since $\delta\mathcal{H}_{\mathrm{GK}}/\delta F_s = H_s^{\mathsf{gy}}$, we have $\mathbf{\Gamma}_{s\bar{s}}^{\mathsf{gy}}(\mathcal{H}_{\mathrm{GK}}) = \boldsymbol{w}_{s\bar{s}}^{\mathsf{gy}}$. Further, since $\boldsymbol{w}_{s\bar{s}}^{\mathsf{gy}} \cdot \mathbb{W}_{s\bar{s}}^{\mathsf{gy}} = 0$, the Hamiltonian functional is a Casimir of the metric bracket

$$(\mathcal{H}_{\mathrm{GK}}, \mathcal{B})_{\mathrm{GK}} = \sum_{s\bar{s}} \frac{c_{s\bar{s}}}{4} \iint \boldsymbol{w}_{s\bar{s}}^{\mathsf{gy}} \cdot \mathbb{W}_{s\bar{s}}^{\mathsf{gy}} \cdot \mathbf{\Gamma}_{s\bar{s}}^{\mathsf{gy}}(\mathcal{B}) d\boldsymbol{z}_s^{\mathsf{gc}} d\bar{\boldsymbol{z}}_{\bar{s}}^{\mathsf{gc}} = 0. \tag{36}$$

Entropy, on the other hand, is a Casimir of the functional Poisson bracket

$$\{\mathcal{B}, \mathcal{S}_{\mathsf{GK}}\}_{\mathsf{GK}} = 0. \tag{37}$$

Thus, with $\mathcal{F}_{\mathrm{GK}} = \mathcal{H}_{\mathrm{GK}} - \mathcal{S}_{\mathrm{GK}}$, the Hamiltonian is conserved

$$\frac{d\mathcal{H}_{\mathsf{GK}}}{dt} = \{\mathcal{H}_{\mathsf{GK}}, \mathcal{F}_{\mathrm{GK}}\}_{\mathrm{GK}} + (\mathcal{H}_{\mathsf{GK}}, \mathcal{F}_{\mathrm{GK}})_{\mathrm{GK}} = 0 \tag{38}$$

Angular momentum conservation law

In axisymmetric $\boldsymbol{B}$, the total toroidal angular momentum

$$\mathcal{P}_\phi = \sum_s \int p_{\phi s}(\boldsymbol{z}) F_s(\boldsymbol{z}) d\boldsymbol{z}_s^{\mathsf{gc}}, \tag{39}$$

with $p_{\phi s}$ the single-particle guiding-center toroidal canonical momentum, is a Casimir of the metric bracket.

Since $\delta\mathcal{P}_\phi/\delta F_s = p_{\phi s}$, we have $\boldsymbol{\Gamma}^{\mathsf{gy}}_{s\bar{s}}(\mathcal{P}_\phi) = \boldsymbol{e}_z \times (\bar{\boldsymbol{y}}_{\bar{s}} - \boldsymbol{y}_s)$ so that

$$(\mathcal{P}_\phi, \mathcal{B})_{\mathrm{GK}} = \sum_{s\bar{s}} \frac{c_{s\bar{s}}}{4} \iint \boldsymbol{e}_z \times (\bar{\boldsymbol{y}}_{\bar{s}} - \boldsymbol{y}_s) \cdot \mathbb{W}^{\mathsf{gy}}_{s\bar{s}} \cdot \boldsymbol{\Gamma}^{\mathsf{gy}}_{s\bar{s}}(\mathcal{B}) d\boldsymbol{z}_s^{\mathsf{gc}} d\bar{\boldsymbol{z}}_{\bar{s}}^{\mathsf{gc}} = 0,$$

which follows from the term$(\bar{\boldsymbol{y}}_{\bar{s}} - \boldsymbol{y}_s)\,\delta^{\mathsf{gy}}_{s\bar{s}}(\boldsymbol{z}, \bar{\boldsymbol{z}})$ in the integrand. Thus, with $\mathcal{F}_{\mathrm{GK}} = \mathcal{H}_{\mathrm{GK}} - \mathcal{S}_{\mathrm{GK}}$, the toroidal angular momentum is conserved

$$\frac{d\mathcal{P}_\phi}{dt} = \{\mathcal{P}_\phi, \mathcal{F}_{\mathrm{GK}}\}_{\mathrm{GK}} + (\mathcal{P}_\phi, \mathcal{F}_{\mathrm{GK}})_{\mathrm{GK}} = 0 \tag{40}$$