

RUHR-UNIVERSITÄT BOCHUM

KINETIC DESCRIPTION OF MAGNETIZED TECHNOLOGICAL PLASMAS

Ralf Peter Brinkmann, Dennis Krüger

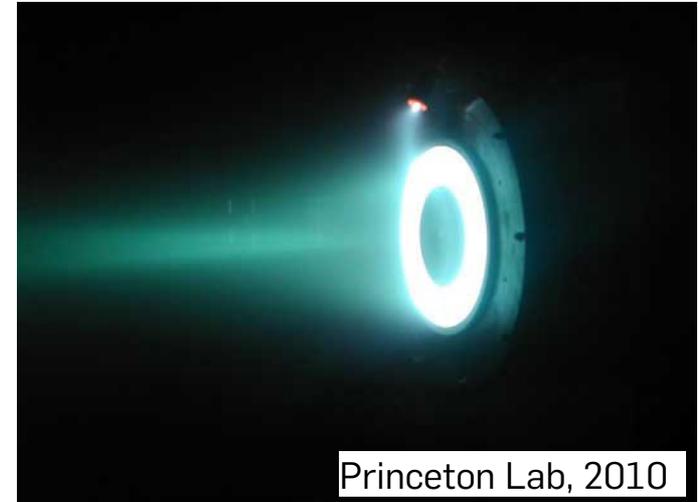
Magnetized low pressure plasmas



HIPIMS



PIAD



Hall Thruster

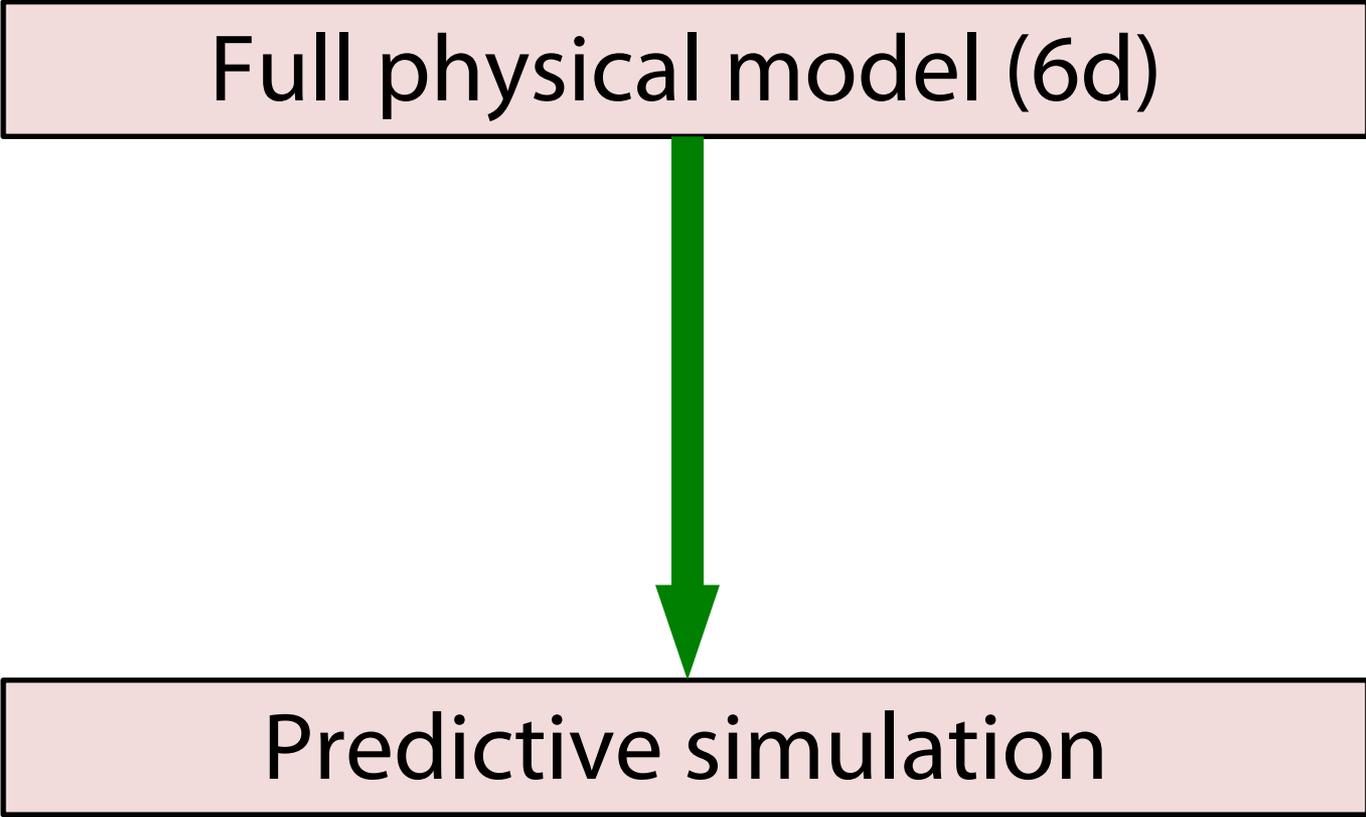
Magnetized low pressure plasmas:

- Basis of many applications
- Complicated physical processes

Modeling of magnetized technological plasmas: Status of the field

Simulation capabilities: Wished for

Full physical model (6d)

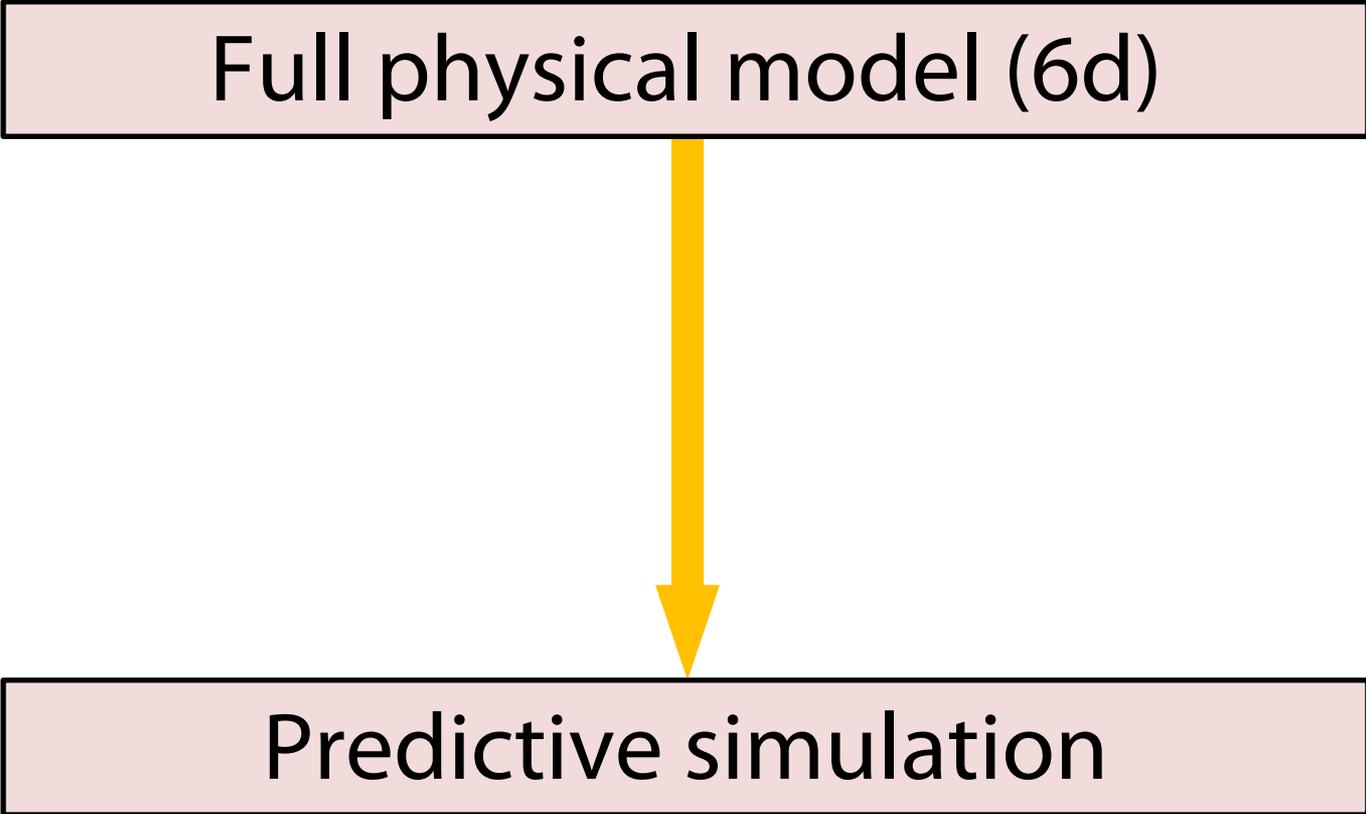


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graph TD; A[Full physical model (6d)] --> B[Predictive simulation]
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Predictive simulation

Simulation capabilities: Current situation

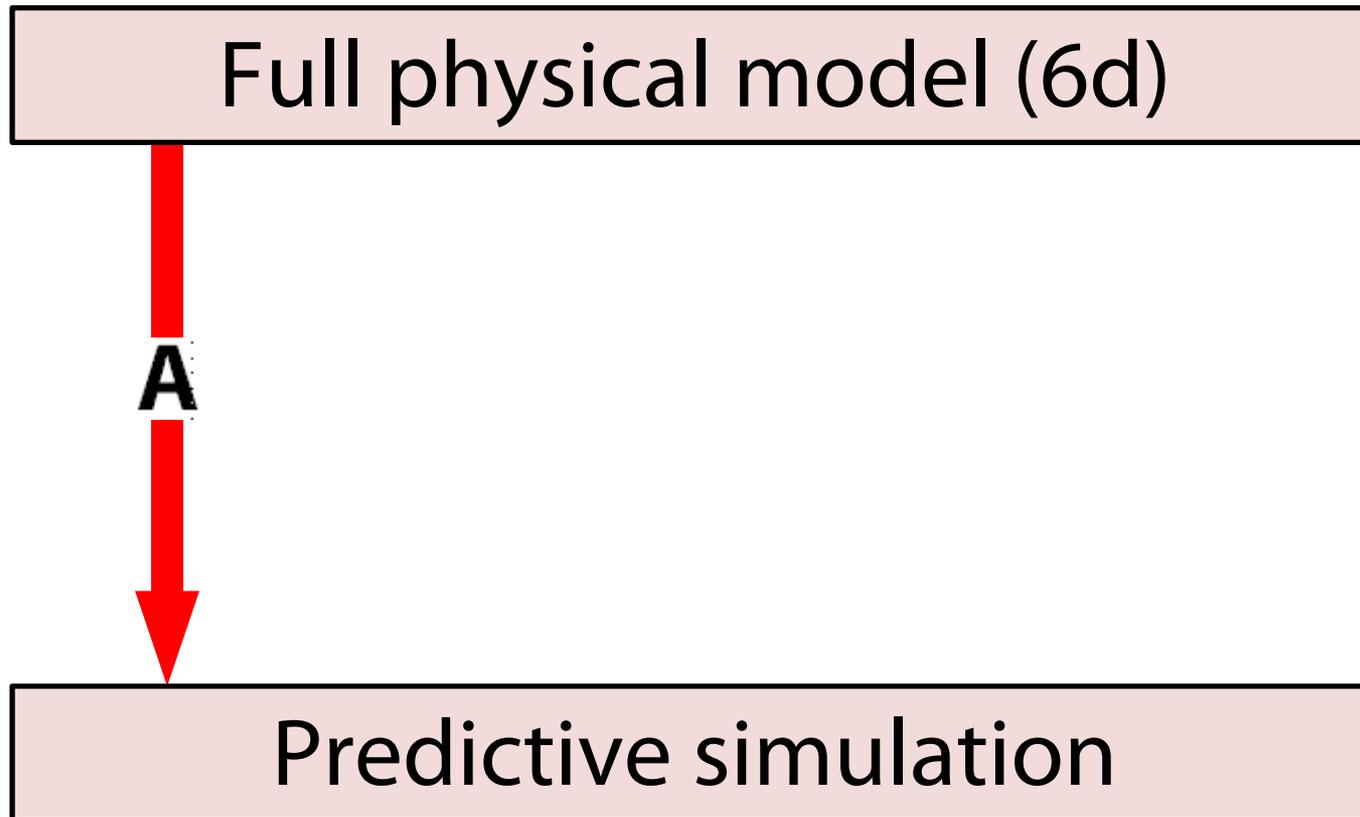
Full physical model (6d)



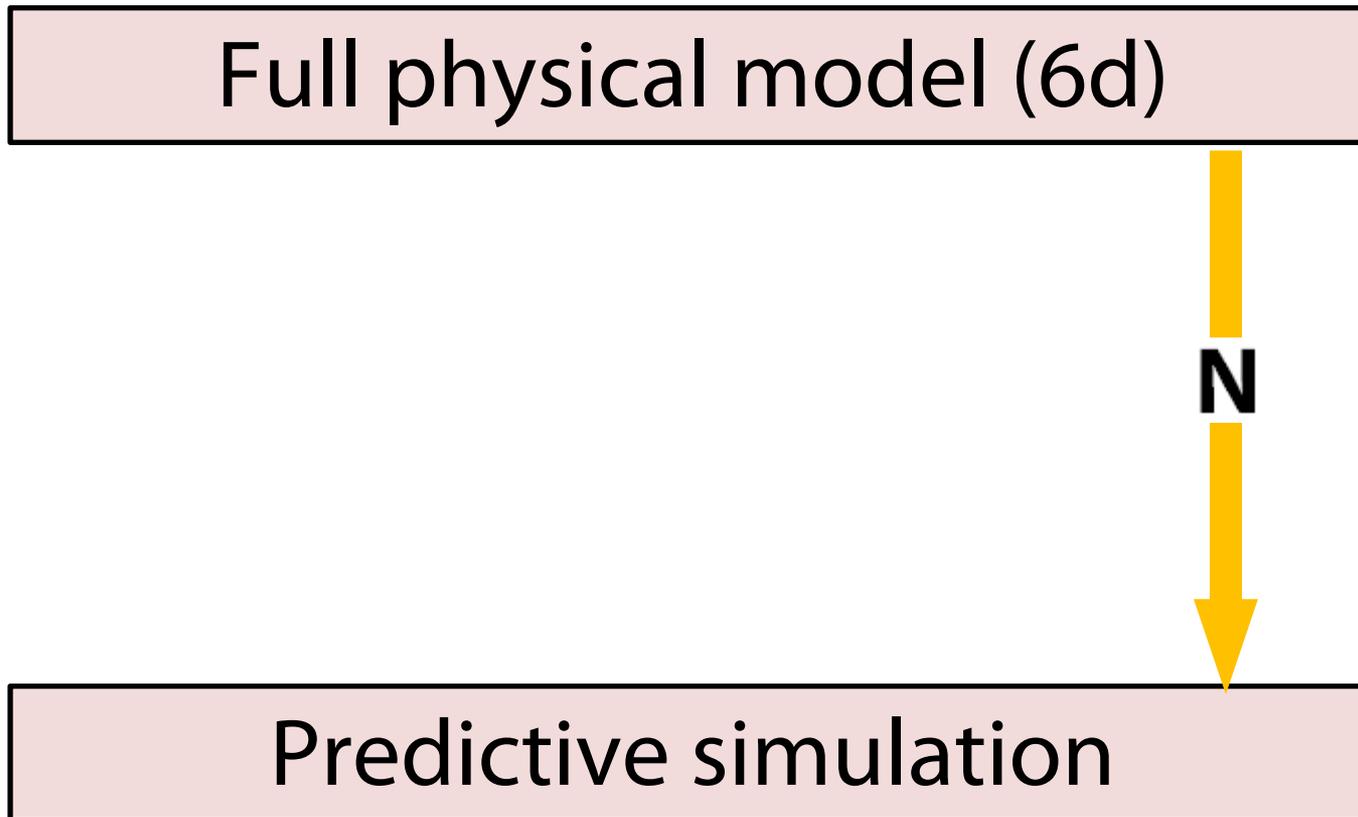
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graph TD; A[Full physical model (6d)] --> B[Predictive simulation]
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Predictive simulation

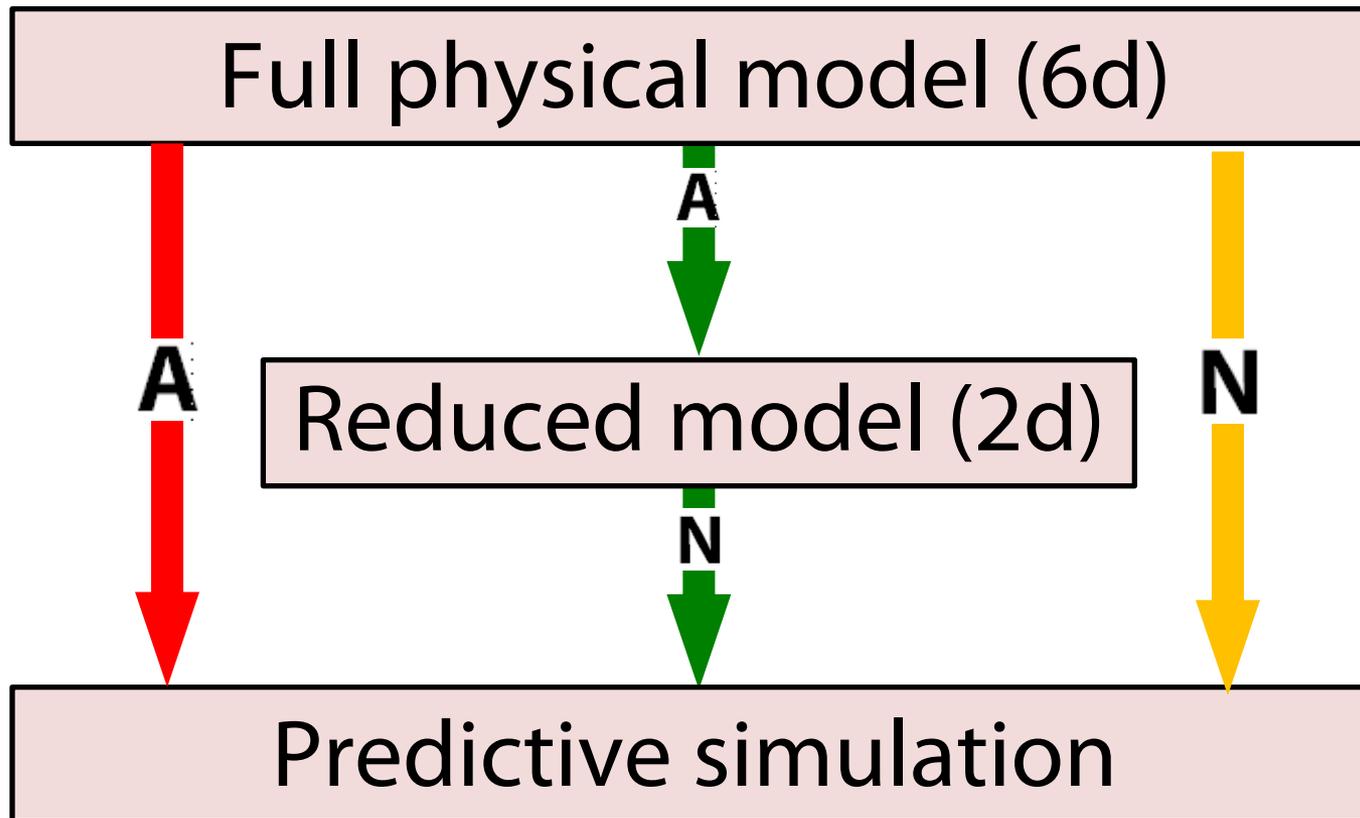
Analytical approaches: Hopeless



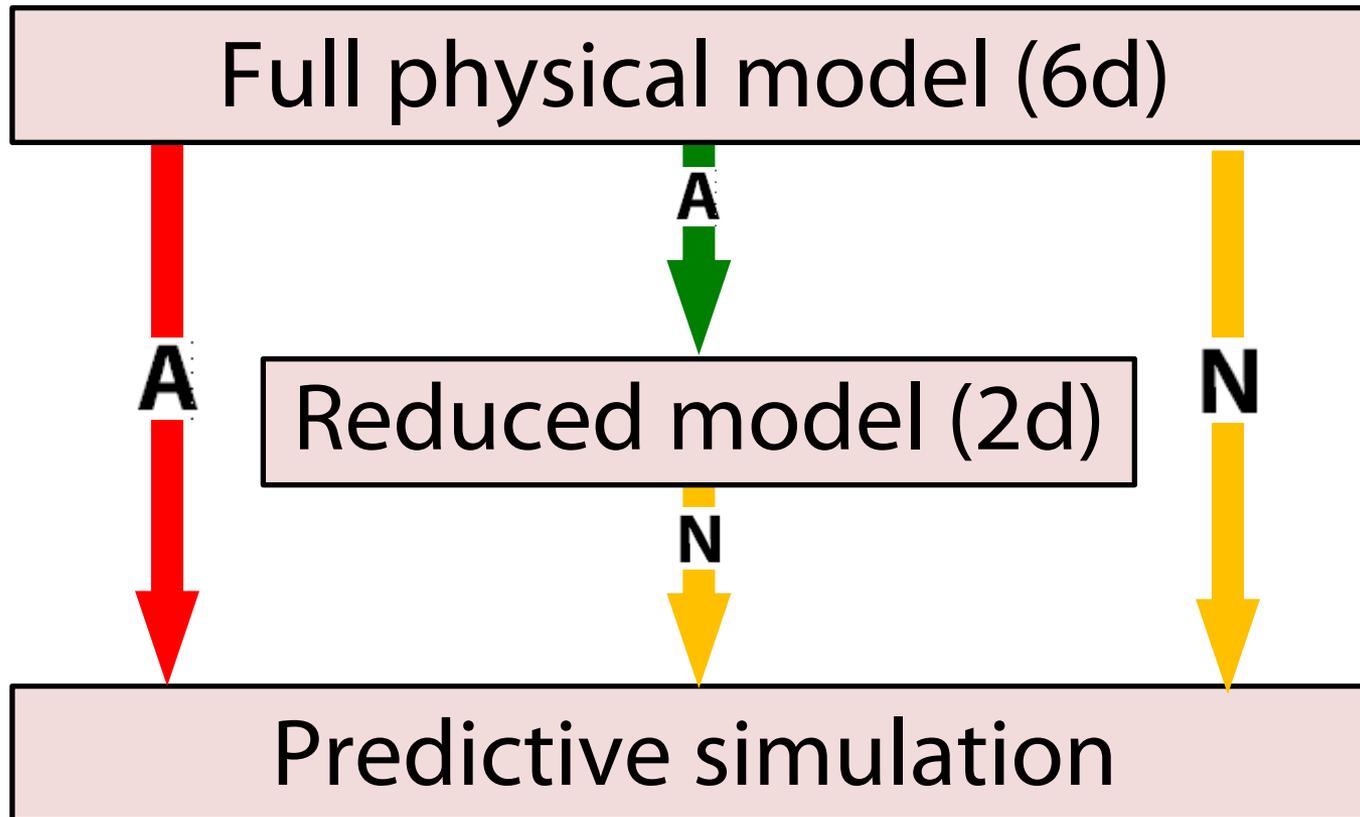
Numerical approaches (PIC): Being worked upon



Our hybrid approach: Wished for

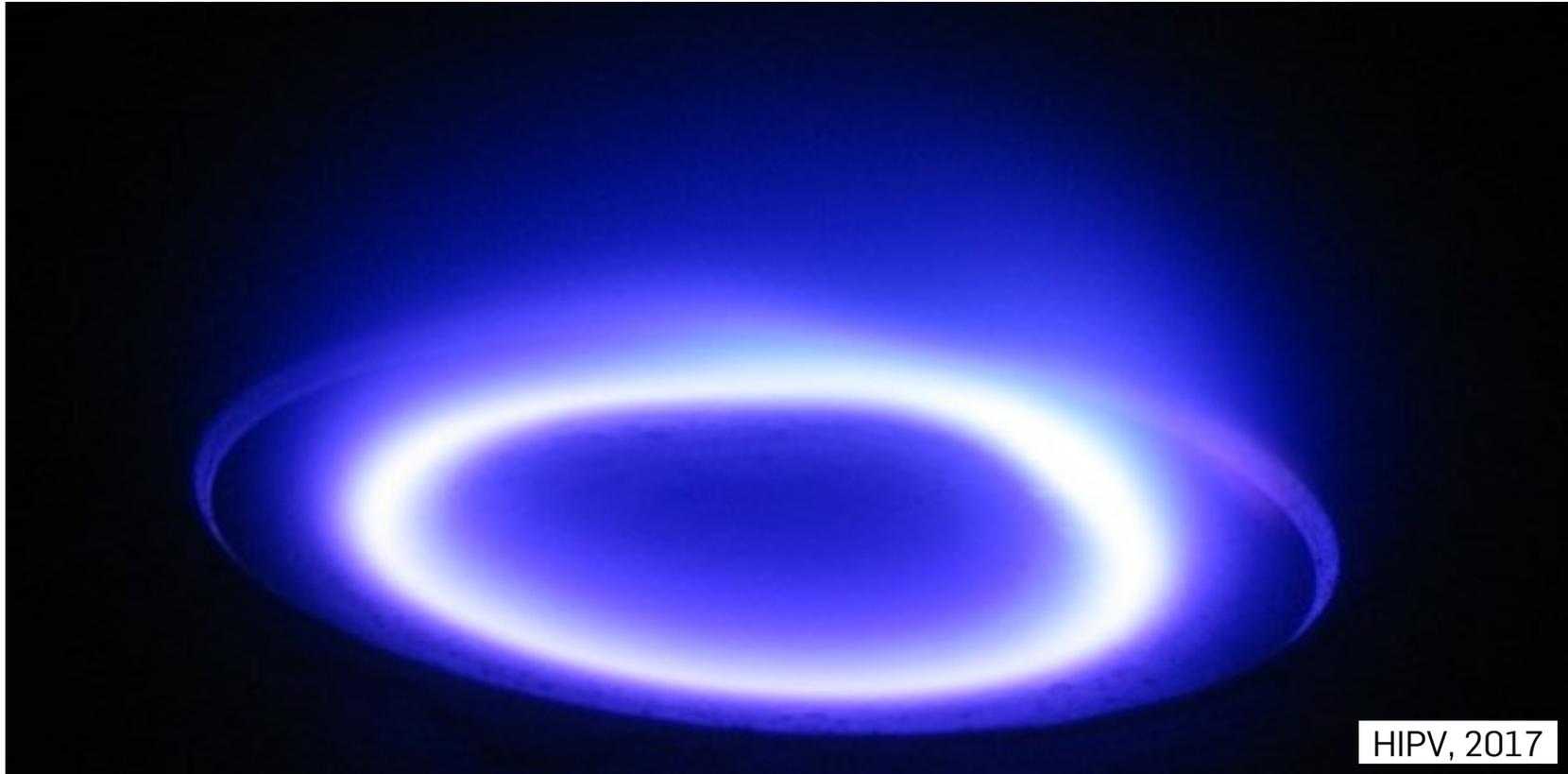


Our hybrid approach, current situation



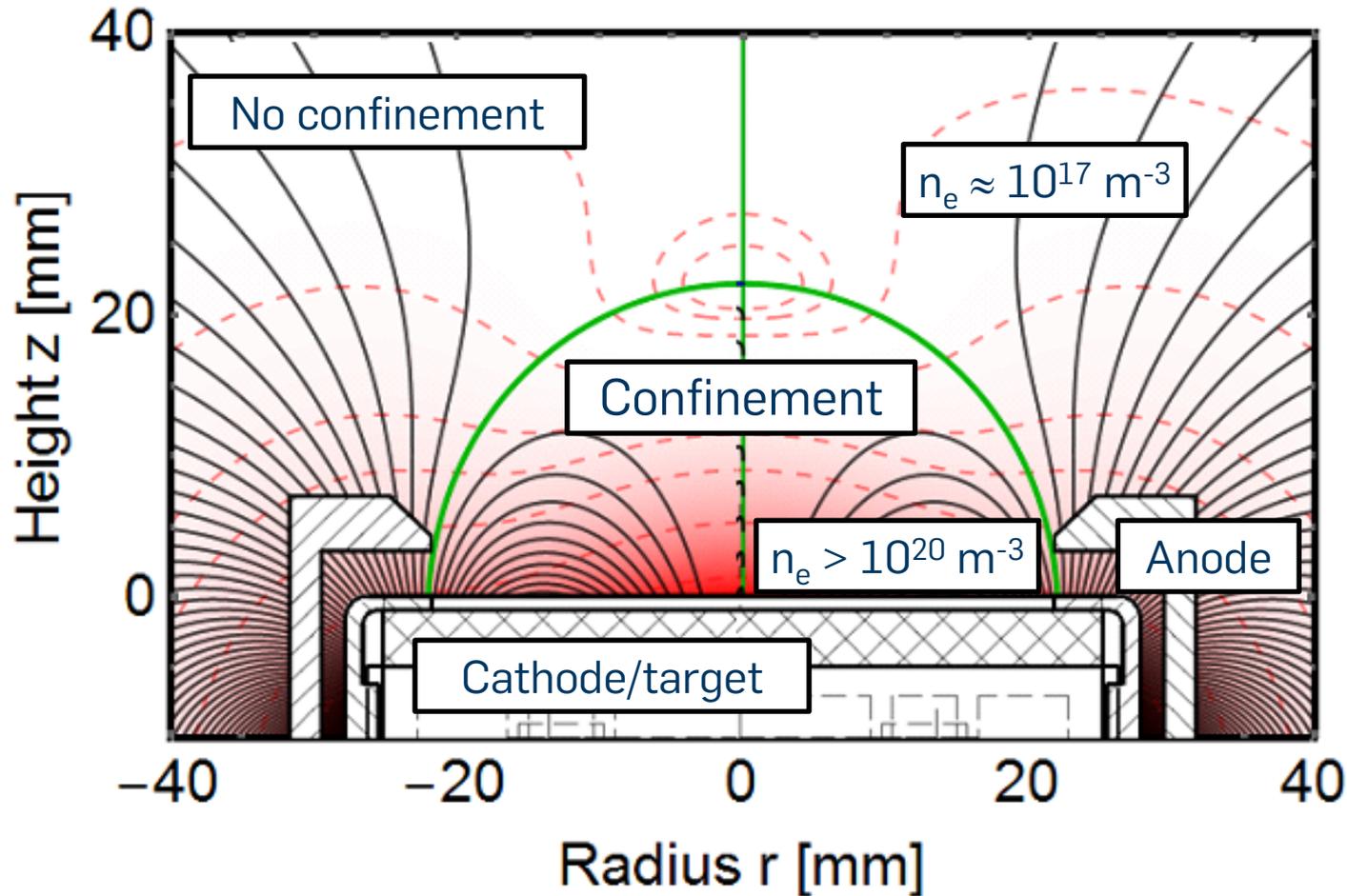
Problems to be solved

Guiding example: Magnetron, as used for HiPIMS



High plasma density in the magnetized region (“race track”).

Structure of a magnetron discharge for HiPIMS



Where are the challenges?

Fusion science offers models to describe magnetized plasmas:

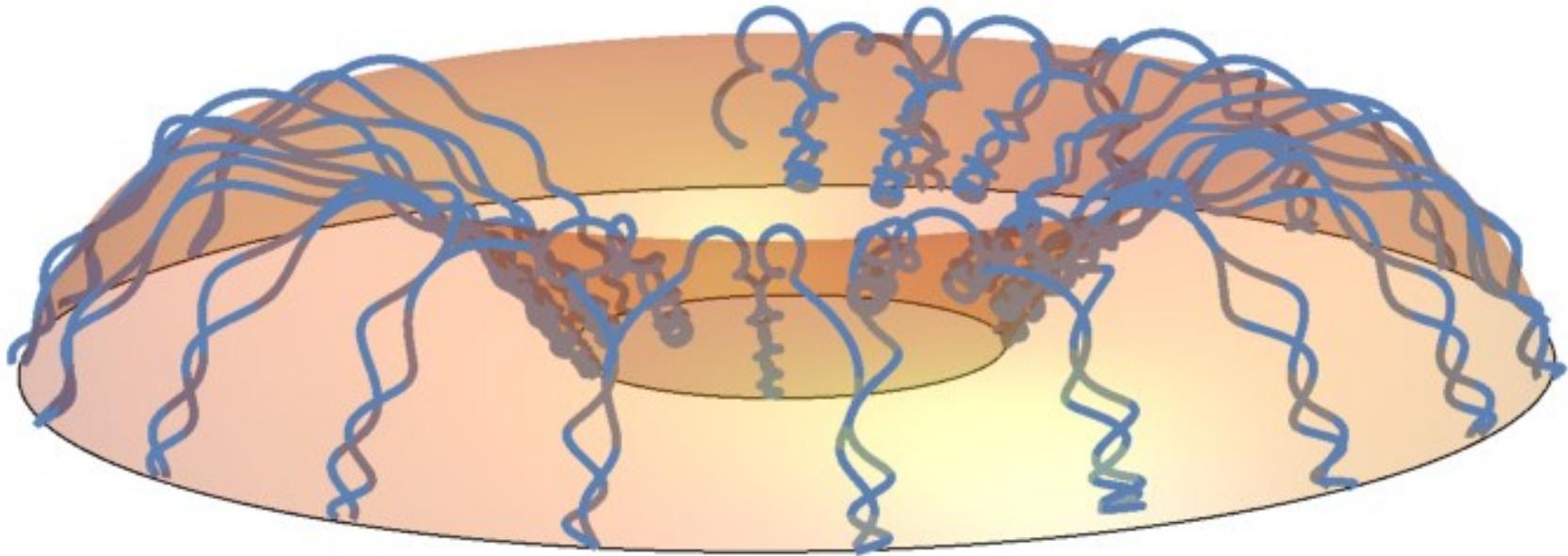
- Drift kinetics, gyro kinetics,

However, low temperature plasmas differ in many ways:

- Only some regions of the discharge are magnetized
- Magnetic field lines have finite length, from wall to wall
- Only electrons are magnetized
- Different groups of electrons may exist (and interact)
- Interaction with the wall and with boundary sheaths is important
- Collisions with neutrals and Coulomb collisions play a role
- Electromagnetic fluctuations have a different spectrum
- Spontaneous symmetry breaking may occur

Strategy: Keep the ideas but start anew from first principles

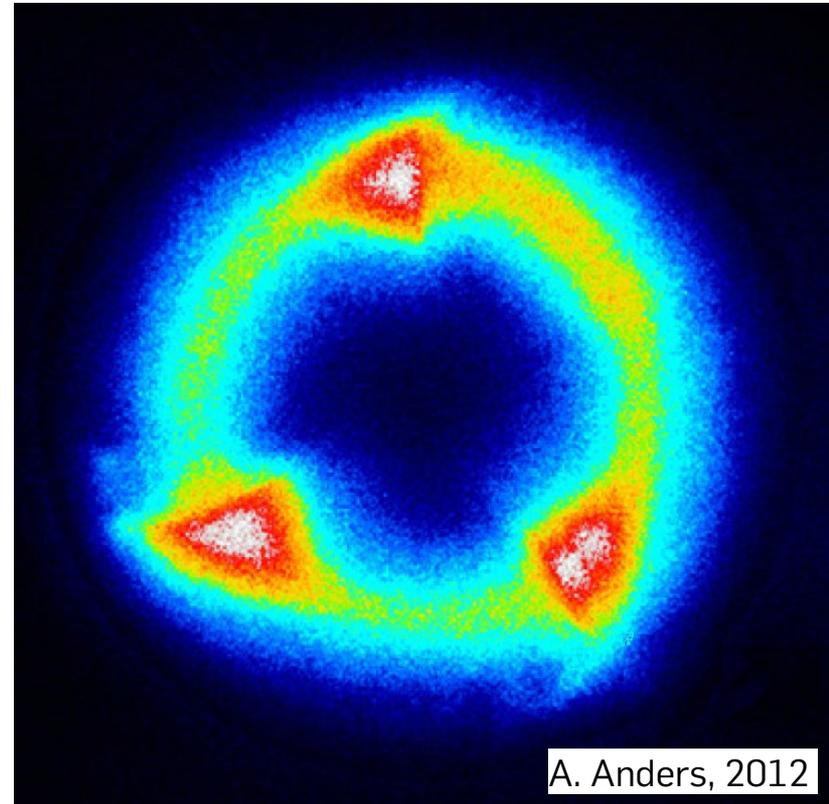
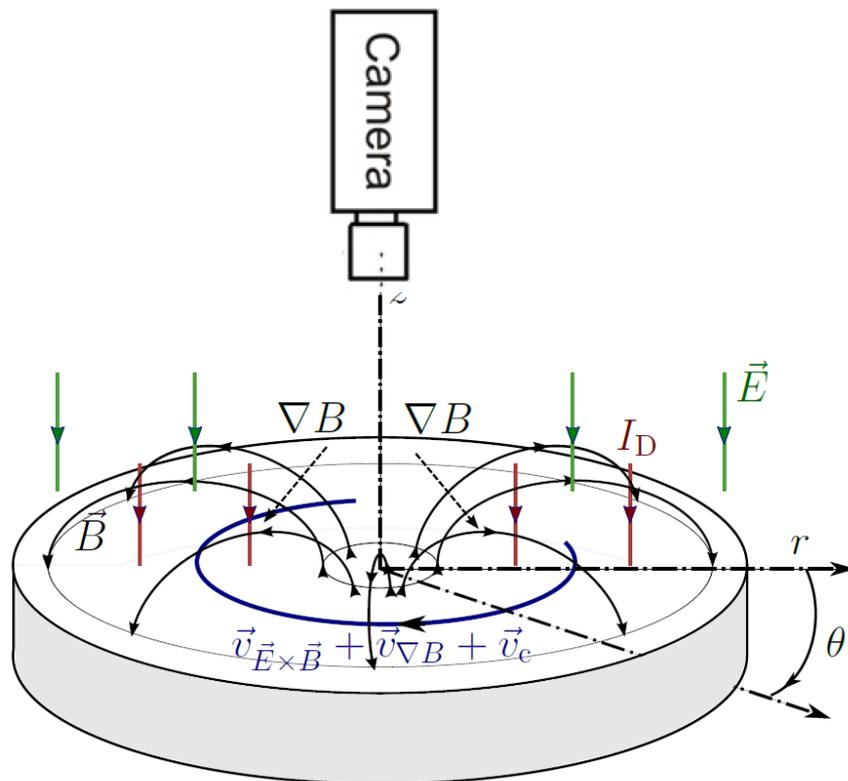
Electron motion in a magnetron (3D visualization)



Motion can be described as a superposition:

- Gyro motion around a magnetic field line
- Bouncing motion between the end points of the field line
- Secular drift in azimuthal direction

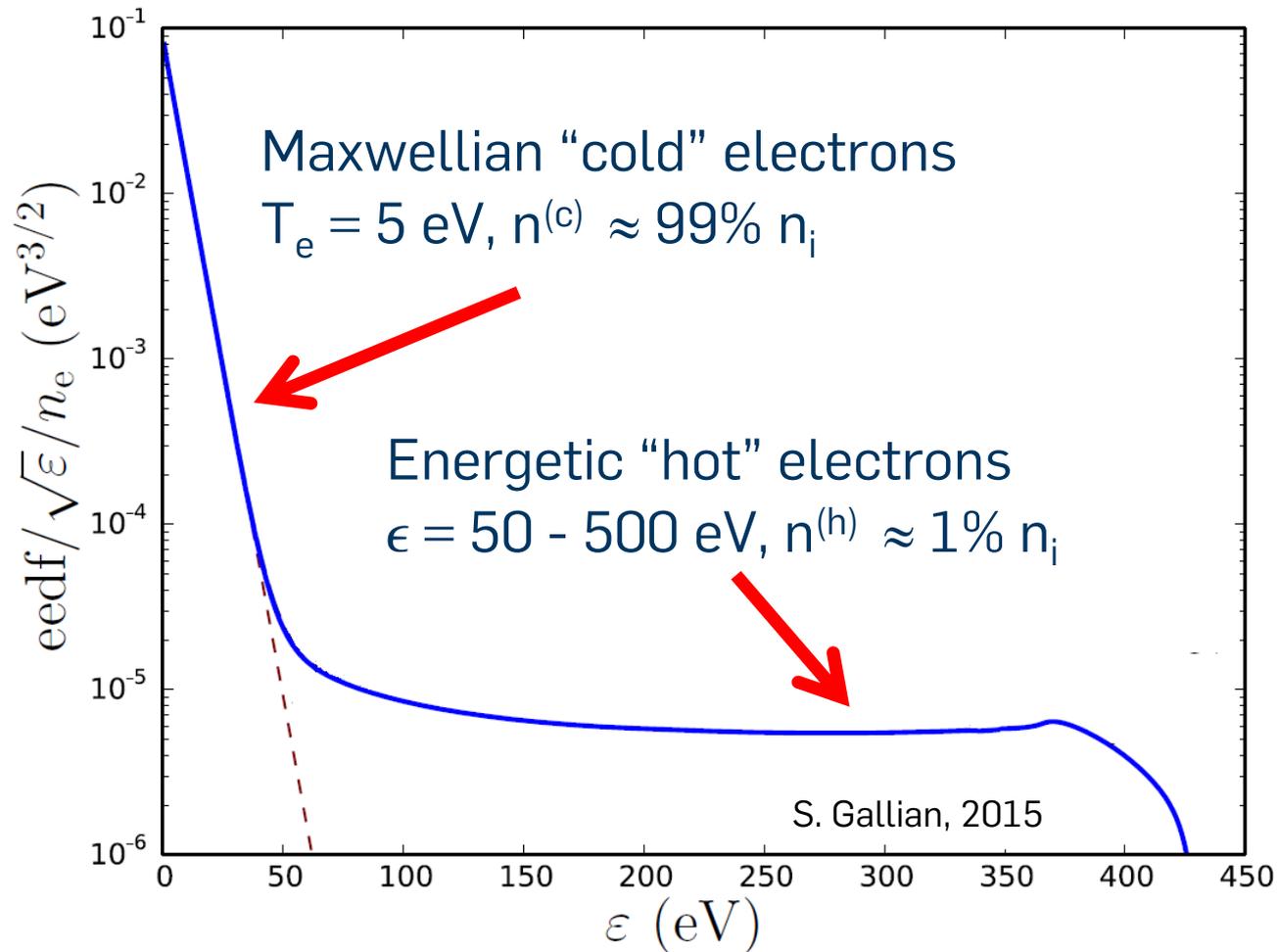
Phenomena of self-organization



Spokes (self-organized rotating ionization zones) break symmetry!

Hot and cold electrons

Structure of the EEDF



Hot and cold electrons are different

Hot electrons:

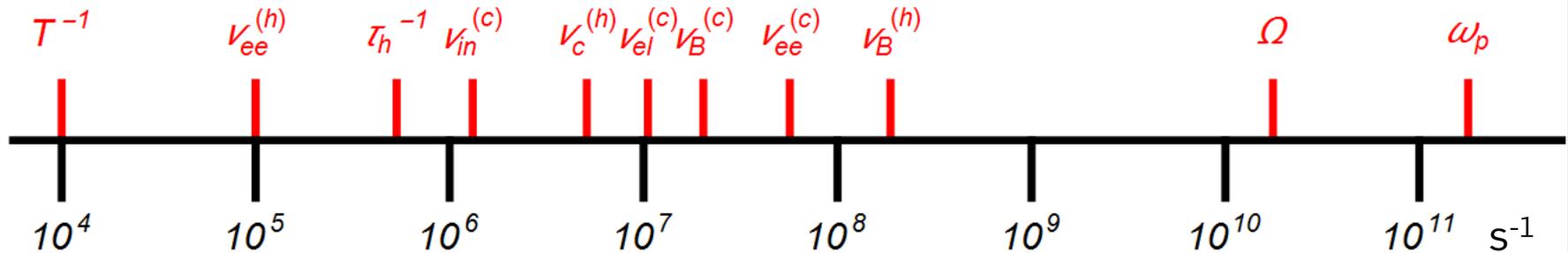
- Born as secondaries at the cathode
- Possibly recaptured by the cathode (at other end of the field line)
- Lose energy by ionization/excitation and friction at cold electrons
- Completely out of thermal equilibrium
- Make up less than 1% of the charge density

Cold electrons:

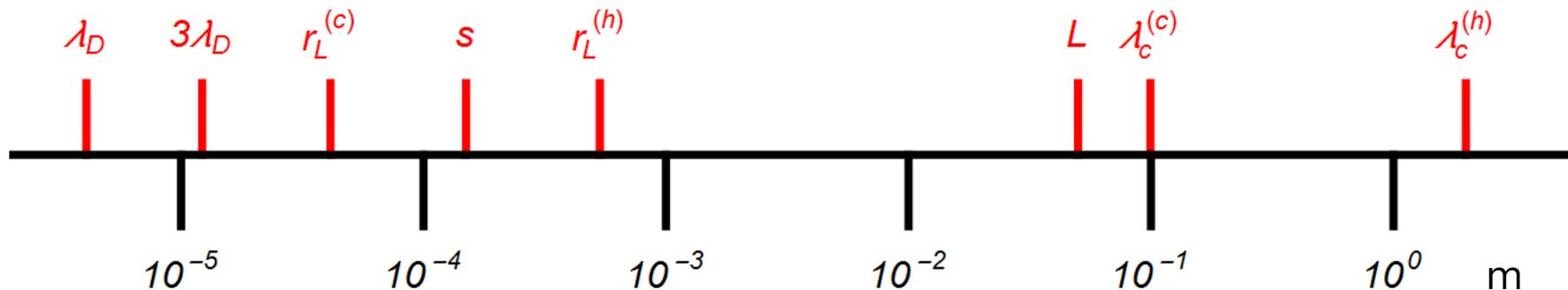
- Created by ionization and from cooled-down hot electrons
- Reflected by the cathode sheath
- Heated by hot electrons and the field, lose energy to neutrals
- Maxwellized by Coulomb interaction (“thermal equilibrium”)
- Make up more than 99% of the electron density

Time and length scales of hot and cold electrons

Characteristic time scales:

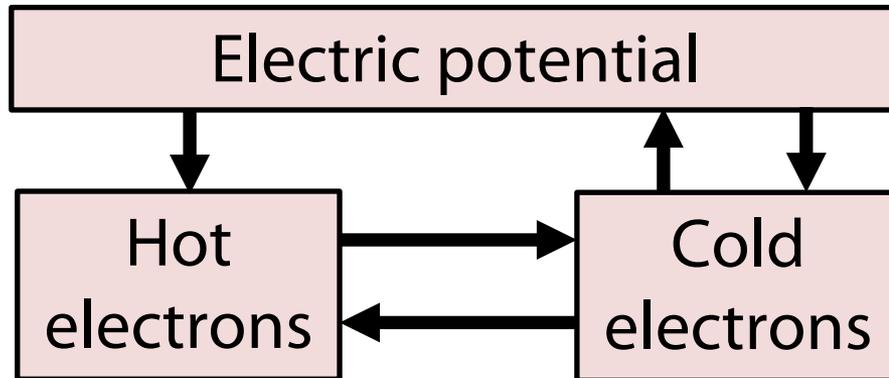


Characteristic length scales:



Again: Hot and cold electrons are different!

Hot and cold electrons must be treated differently



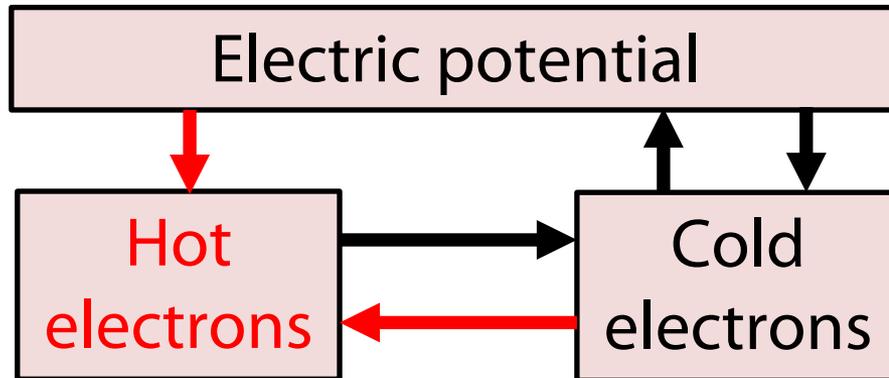
Hot electrons experience the field and friction from the cold ones:

$$\langle f_h, f \rangle_{ee} = \frac{e^4 n_e \ln \Lambda}{4\pi \epsilon_0^2 m_e^2} \frac{\partial}{\partial \mathbf{v}} \cdot \left(\frac{\mathbf{v}}{|\mathbf{v}|^3} f_h(\mathbf{v}) \right)$$

Cold electrons are heated by the hot ones and interact with the field:

$$\langle f, f_h \rangle_{ee} = \frac{e^4 \ln \Lambda}{12\pi \epsilon_0^2 m_e^2} \int \frac{1}{|\mathbf{v}'|} f_h(\mathbf{v}') dv'^3 \frac{\partial^2 f}{\partial \mathbf{v}^2}$$

Cold and hot electrons must be treated differently



**Hot electrons:
Monte Carlo-simulation
with given potential**

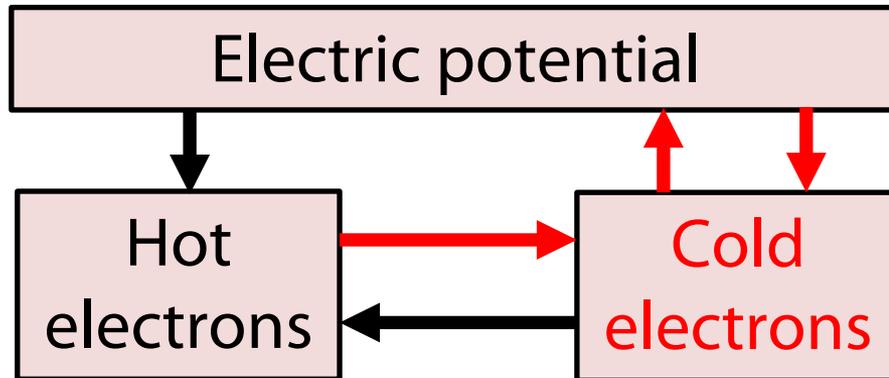
Hot electrons experience the field and friction from the cold ones:

$$\langle f_h, f \rangle_{ee} = \frac{e^4 n_e \ln \Lambda}{4\pi \epsilon_0^2 m_e^2} \frac{\partial}{\partial \mathbf{v}} \cdot \left(\frac{\mathbf{v}}{|\mathbf{v}|^3} f_h(\mathbf{v}) \right)$$

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Cold and hot electrons must be treated differently



Cold electrons:
Kinetic model with
imposed quasi-neutrality

Hot electrons experience the field and friction from the cold ones:

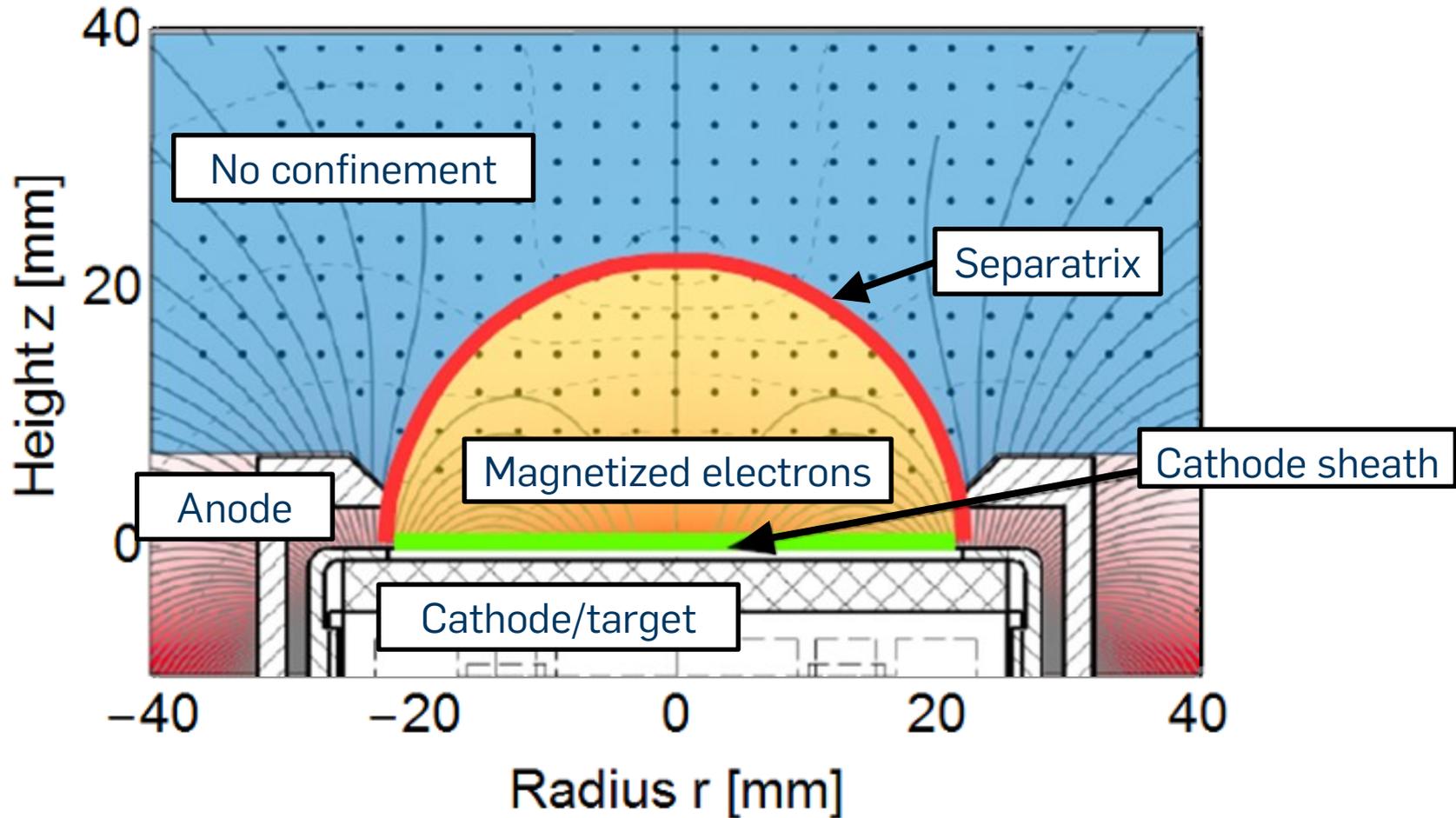
$$\langle f_h, f \rangle_{ee} = \frac{e^4 n_e \ln \Lambda}{4\pi \epsilon_0^2 m_e^2} \frac{\partial}{\partial \mathbf{v}} \cdot \left(\frac{\mathbf{v}}{|\mathbf{v}|^3} f_h(\mathbf{v}) \right)$$

Cold electrons are heated by the hot ones and interact with the field:

$$\langle f, f_h \rangle_{ee} = \frac{e^4 \ln \Lambda}{12\pi \epsilon_0^2 m_e^2} \int \frac{1}{|\mathbf{v}'|} f_h(\mathbf{v}') dv'^3 \frac{\partial^2 f}{\partial \mathbf{v}^2}$$

Kinetic description of the cold electrons

Domain and boundaries of the cold electron model



Kinetic theory for the cold electrons

Dynamic equation for the cold electron distribution function:

$$\begin{aligned} \frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{q}{m} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial f}{\partial \mathbf{v}} \\ = \langle f \rangle_{\text{el}} + \langle f \rangle_{\text{in}} + \langle f \rangle_{\text{ei}} + \langle f, f \rangle_{\text{ee}} + \langle f_{\text{h}}, f \rangle_{\text{ee}} \end{aligned}$$

Left side of the equation: Deterministic part

- Evolution due to spatial gradients and electromagnetic forces (magnetic field given, electric field from quasi-neutrality)

Right side of the equation: Stochastic part

- Elastic and inelastic collisions
- Coulomb interaction with ions and other cold electrons
- Coulomb interaction (heating) by hot electrons

Scale relations for the cold electrons

Two length scales are considered:

- Macroscopic scale: System size L , mean free path λ
- Microscopic scale: Gyro radius r_L of the cold electrons
- Smallness parameter: $\delta = r_L/L \approx 0.01 \ll 1$

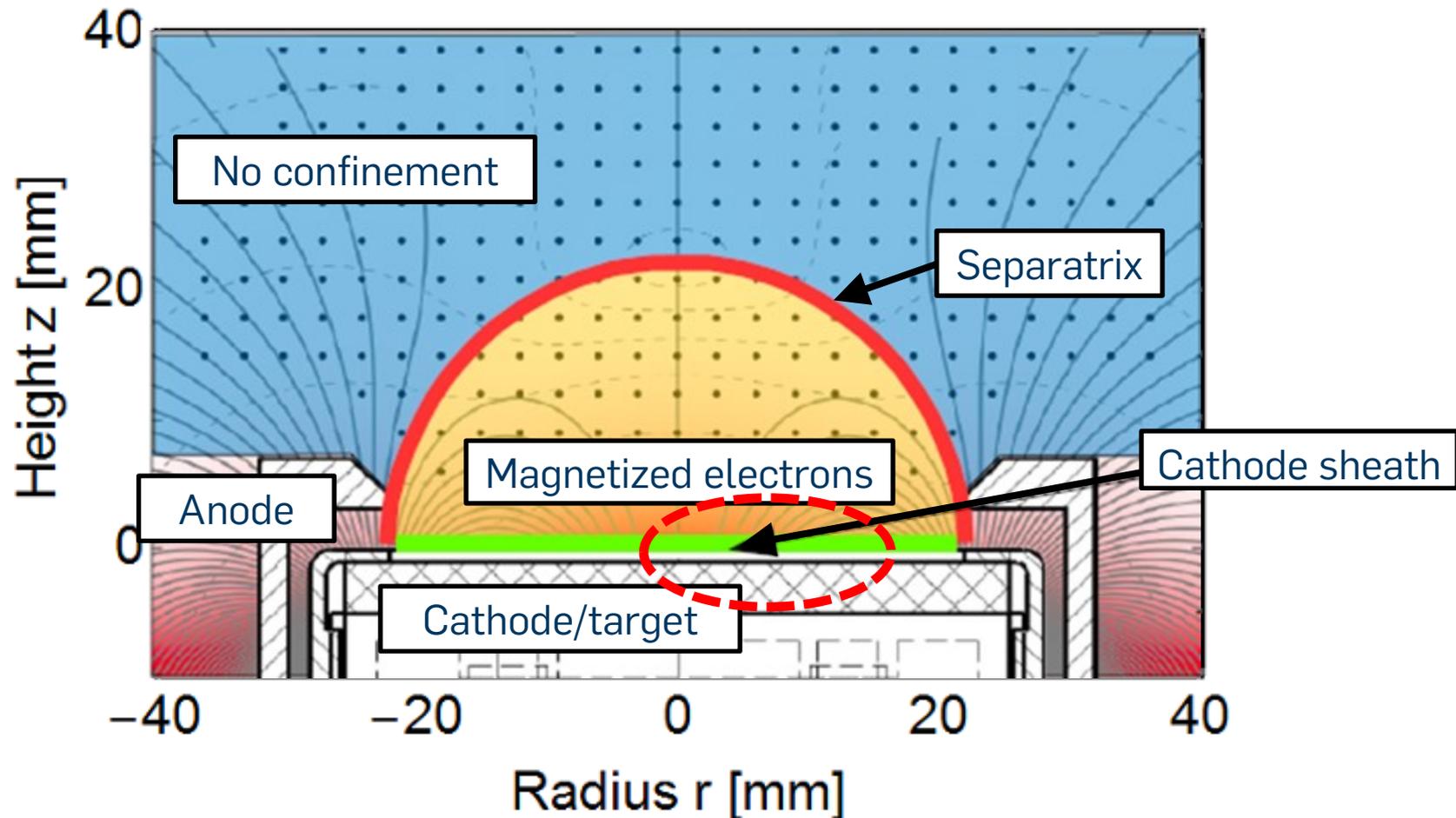
Resulting time scales (with azimuthal mode number $m \approx 10$):

- Gyro motion $\Omega \approx v/r_L \approx 2\pi \times 1 \text{ GHz}$
- Bouncing/collision $v/L \approx \nu \sim \delta \Omega \approx 2\pi \times 10 \text{ MHz}$
- ExB and other drifts $m(E/B)/L \sim m \delta^2 \Omega \approx 2\pi \times 1 \text{ MHz}$
- Collisional diffusion $m^2 \nu (r_L/L)^2 \sim m^2 \delta^3 \Omega \approx 2\pi \times 100 \text{ KHz}$

► To capture the relevant physics, all four time scales are needed!

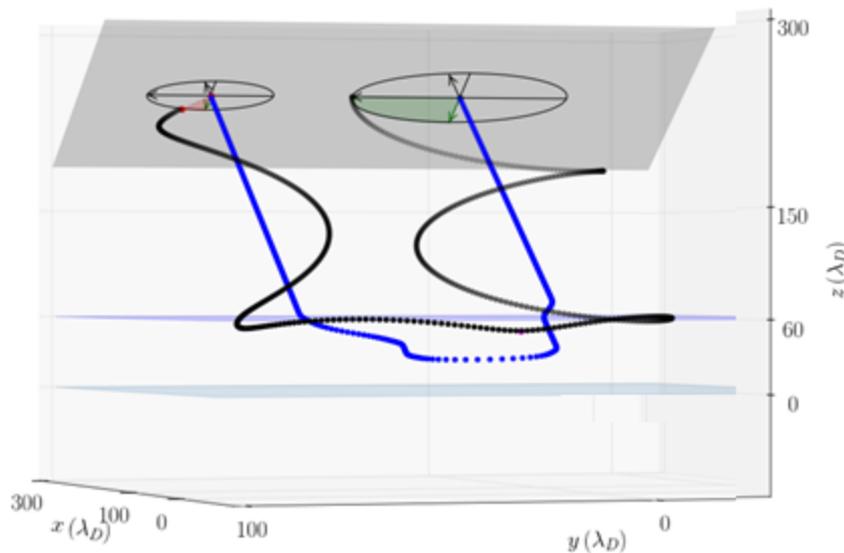
Boundary conditions at the cathode sheath

Boundary conditions at the cathode sheath

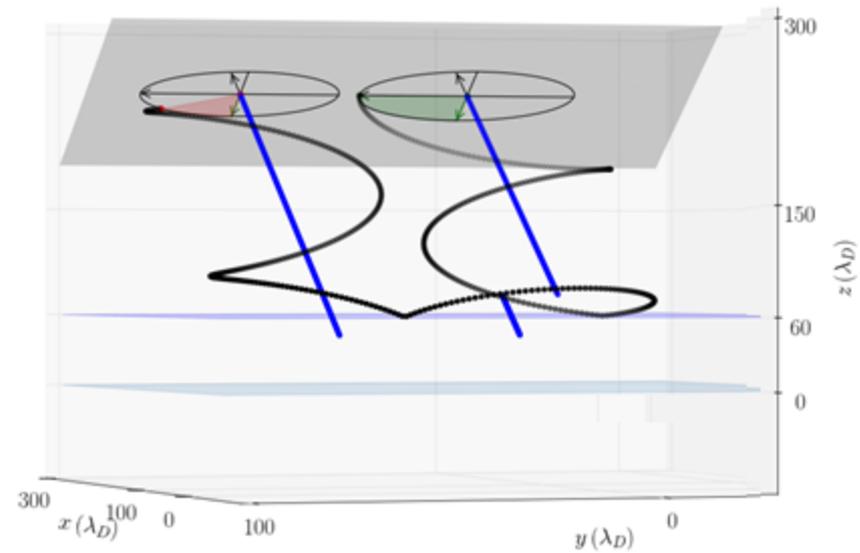


Interaction with the cathode sheath

Cold electrons are reflected from the cathode sheath:



Spatially resolved (Bohm)



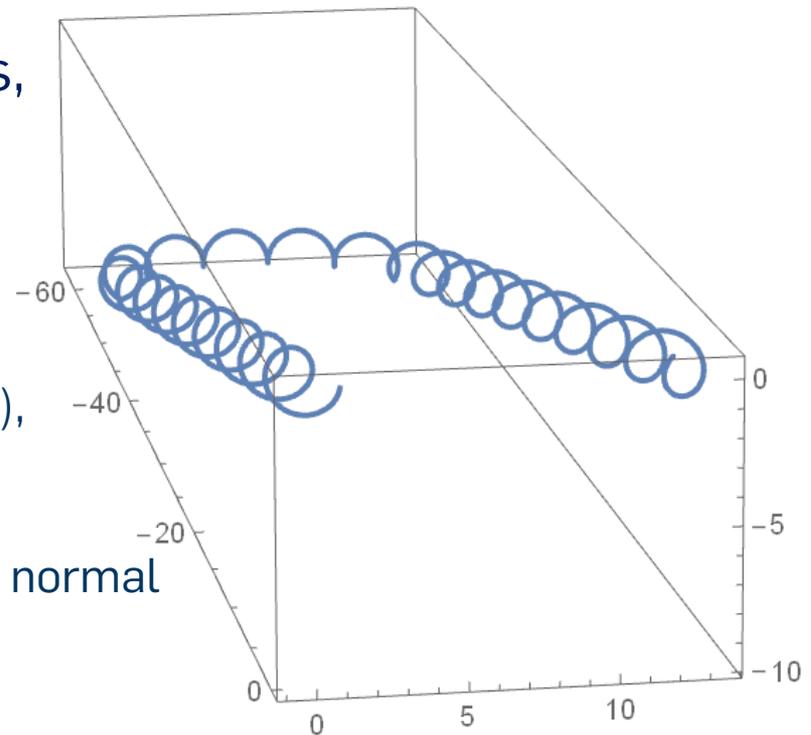
Spatially not resolved (hard wall)

Numerical tests confirm: The hard wall model (specular reflection) is a good approximation to the spatially resolved Bohm model.

Local model of gyration and specular reflection

For a local model, neglect collisions, curvature, and electric field.

Cartesian coordinates (x,y,z) ,
hard wall in plane $z=0$,
magnetic field in x - z -plane,
inclination γ with respect to normal



Scenario of the local model:

- An incoming electron moves on a helix around its field line
- One or multiple specular reflections occur at the sheath
- The outgoing electron moves freely around a different field line

Local kinetic equation with boundary conditions

Kinetic equation Cartesian coordinates:

$$\frac{\partial f}{\partial t} + v_x \frac{\partial f}{\partial x} + v_y \frac{\partial f}{\partial y} + v_z \frac{\partial f}{\partial z} - \Omega v_y \cos \gamma \frac{\partial f}{\partial v_x} + \Omega (v_x \cos \gamma - v_z \sin \gamma) \frac{\partial f}{\partial v_y} + \Omega v_y \sin \gamma \frac{\partial f}{\partial v_z} = 0$$

Specular boundary conditions at $z=0$:

$$f(x, y, z, v_x, v_y, v_z, t) \Big|_{z=0} = f(x, y, z, v_x, v_y, -v_z, t) \Big|_{z=0}$$

In Cartesian coordinates (x,y,z) , the kinetic equation is complicated, but the boundary conditions are transparent.

System of local gyro coordinates

To describe the gyration and the specular interaction, define:

$$\hat{X} = x - z \tan \gamma + v_y / (\Omega \cos \gamma)$$

$$\hat{Y} = y - v_x / (\Omega \cos \gamma)$$



Coordinates of the
field line base point

$$s = z / \cos \gamma - \tan \gamma v_y / \Omega$$

$$\epsilon = \frac{1}{2} (v_x^2 + v_y^2 + v_z^2)$$

Guiding center location

Kinetic energy

$$\chi = \arccos \left(\frac{v_z \cos \gamma + v_x \sin \gamma}{\sqrt{v_x^2 + v_y^2 + v_z^2}} \right)$$



Gyro elements:
Pitch angle / gyro phase

$$\phi = \arctan (v_x \cos \gamma - v_z \sin \gamma, v_y)$$

System of local gyro coordinates

To describe the gyration and the specular interaction, define:

$$\hat{X} = x - z \tan \gamma + v_y / (\Omega \cos \gamma)$$

$$\hat{Y} = y - v_x / (\Omega \cos \gamma)$$



Constants of gyro motion
and sheath reflection

$$s = z / \cos \gamma - \tan \gamma v_y / \Omega$$

Shows uniform motion

$$\epsilon = \frac{1}{2} (v_x^2 + v_y^2 + v_z^2)$$

Constant of motion

$$\chi = \arccos \left(\frac{v_z \cos \gamma + v_x \sin \gamma}{\sqrt{v_x^2 + v_y^2 + v_z^2}} \right)$$



Simple gyro dynamics
but complicated form
of the sheath interaction

$$\phi = \arctan (v_x \cos \gamma - v_z \sin \gamma, v_y)$$

Kinetic equation in local gyro coordinates

In the local gyro coordinates, the kinetic equation simplifies:

$$\frac{\partial f}{\partial t} + \sqrt{2\epsilon} \cos \chi \frac{\partial f}{\partial s} - \Omega \frac{\partial f}{\partial \phi} = 0$$

General stationary solution:

$$f(s, \epsilon, \chi, \phi) = F\left(\epsilon, \chi, \phi + s\Omega/\sqrt{2\epsilon} \sin \chi\right)$$

Distributions functions that have structure on the gyro phase ϕ are subject to fast phase mixing:

$$f(s, \epsilon, \chi, \phi) \rightarrow \bar{f}(\epsilon, \chi) := \frac{1}{2\pi} \int_0^{2\pi} f(s, \epsilon, \chi, \phi) d\phi$$

Assumption: Incoming electrons have a gyro-invariant distribution. (They have travelled a distance far larger than $\sqrt{2\epsilon}/\Omega$.)

Specular reflection in local gyro coordinates

The specular reflection law gets more complicated:

$$\chi_i^+ = \arccos(\sin 2\gamma \sin \chi_i^- \cos \phi_i^- - \cos 2\gamma \cos \chi_i^-)$$

$$\phi_i^+ = \arctan(\sin 2\gamma \cos \chi_i^- + \cos 2\gamma \sin \chi_i^- \cos \phi_i^-, \sin \chi_i^- \sin \phi_i^-)$$

However, a numerical construction is possible:

- Take an incoming electron with given gyro elements (χ_{in}, ϕ_{in}) , calculated in reference to the formal sheath plane $s=0$.
- Follow the electron in its (possibly multiple) sheath interactions until it has become an outgoing electron.
- Calculate the gyro elements (χ_{out}, ϕ_{out}) of the outgoing electron in reference to the formal sheath plane $s=0$.

The mapping $(\chi_{in}, \phi_{in}) \rightarrow (\chi_{out}, \phi_{out})$ defines the collision operator T .

Properties of the sheath collision operator

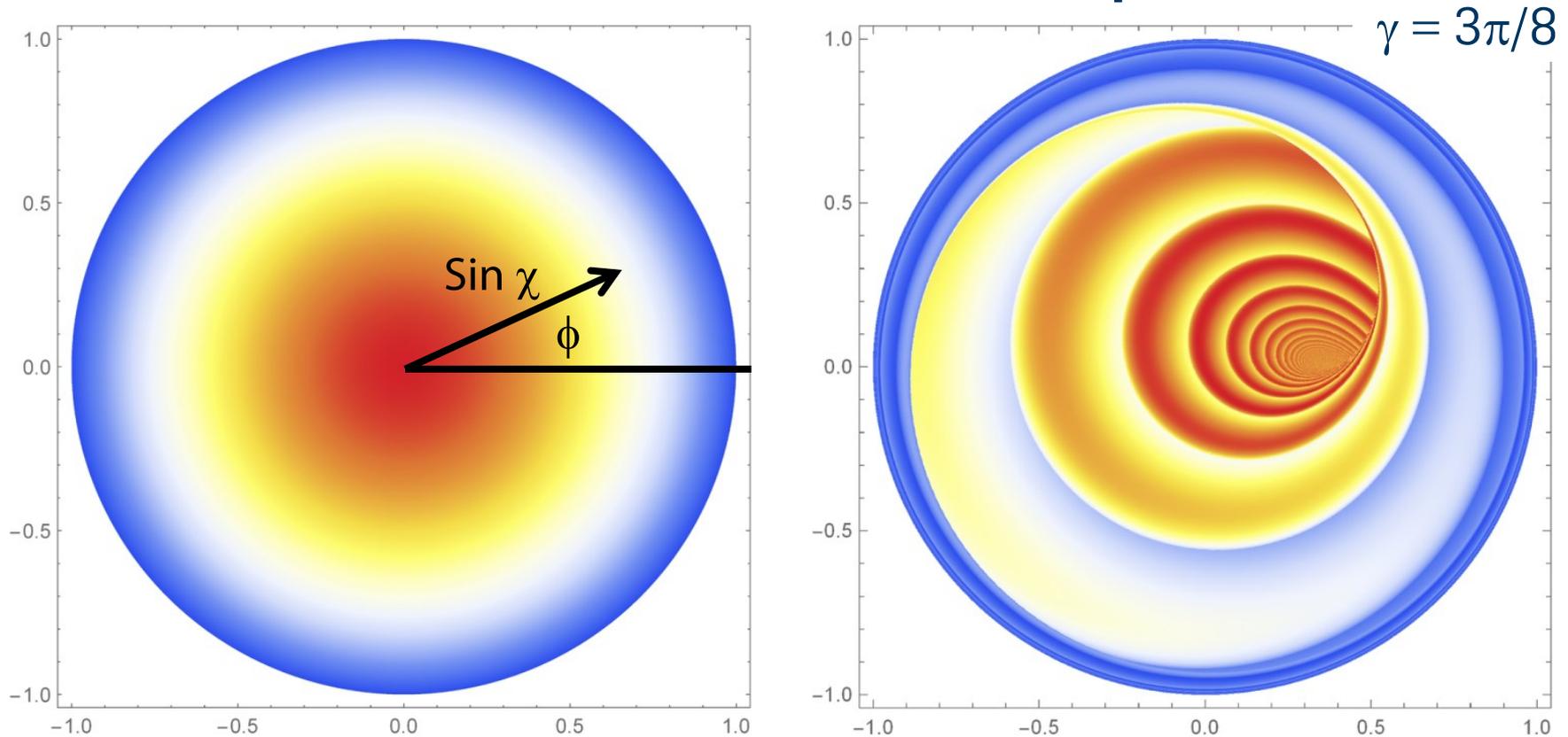
The collision operator T has a number of special properties:

- It is regular and invertible (in fact, it is its own inverse).
- It is everywhere continuous but not everywhere differentiable.
- In points where it is differentiable, the Jacobian is given by

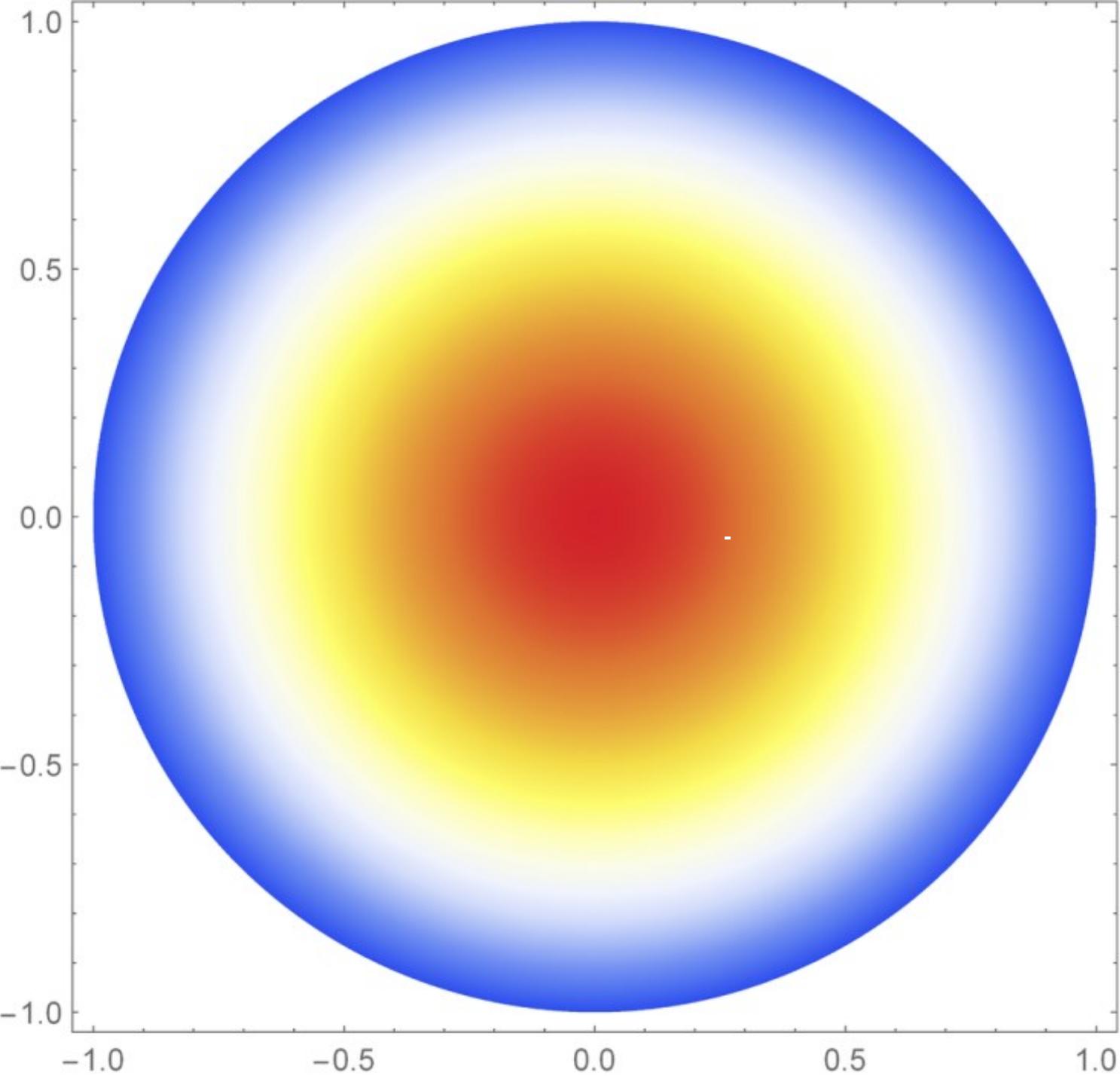
$$\begin{vmatrix} \frac{\partial \chi_{\text{out}}}{\partial \chi_{\text{in}}} & \frac{\partial \phi_{\text{out}}}{\partial \chi_{\text{in}}} \\ \frac{\partial \chi_{\text{out}}}{\partial \phi_{\text{in}}} & \frac{\partial \phi_{\text{out}}}{\partial \phi_{\text{in}}} \end{vmatrix} = \frac{\sin \chi_{\text{in}} \cos \chi_{\text{in}}}{\sin \chi_{\text{out}} \cos \chi_{\text{out}}}$$

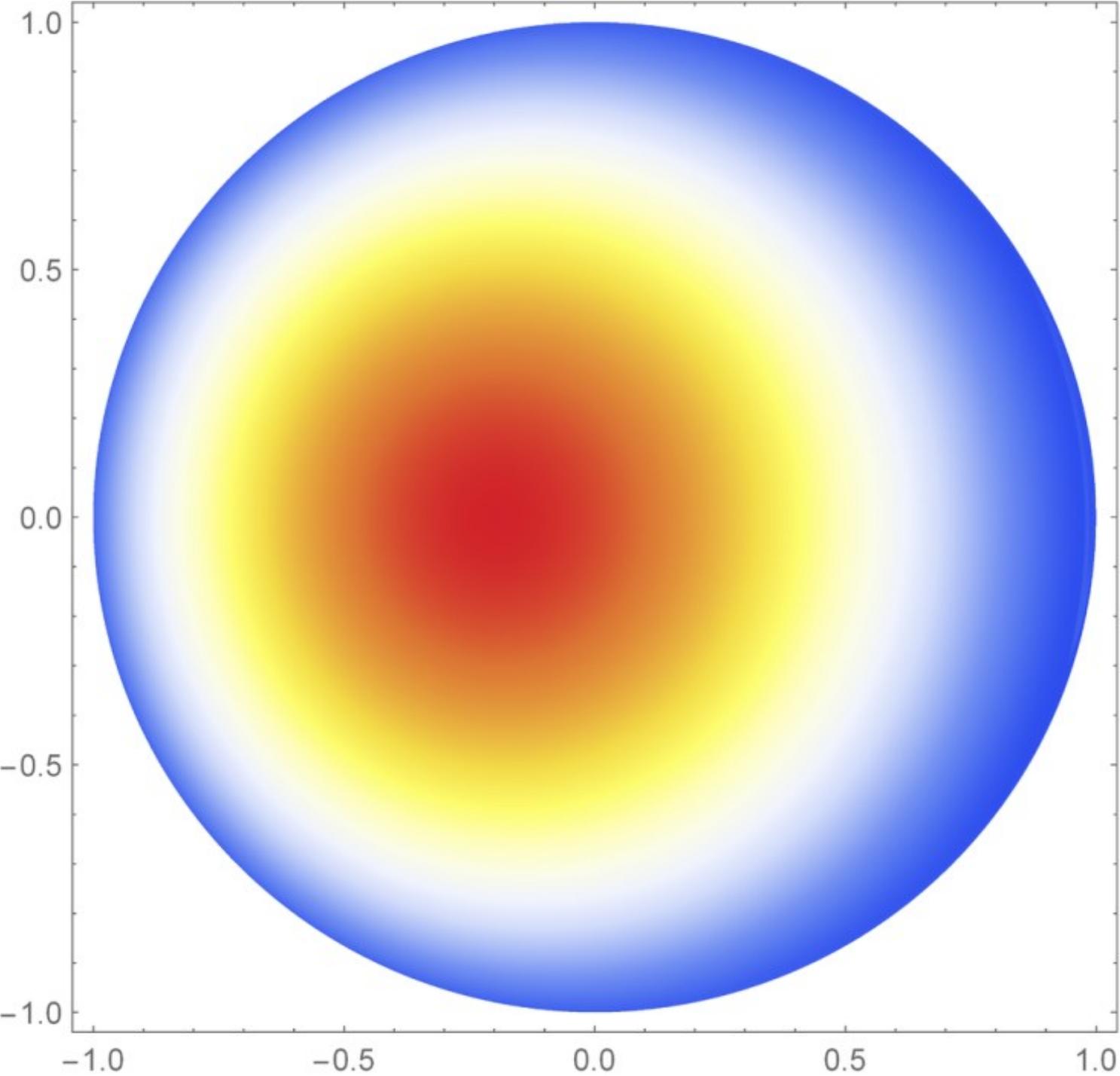
- Particle flux, energy flux, and free energy flux are conserved
- Incoming isotropic distributions yield isotropic outgoing ones
- Incoming gyro-invariant but anisotropic regular distributions are mapped onto outgoing distributions with gyro structure

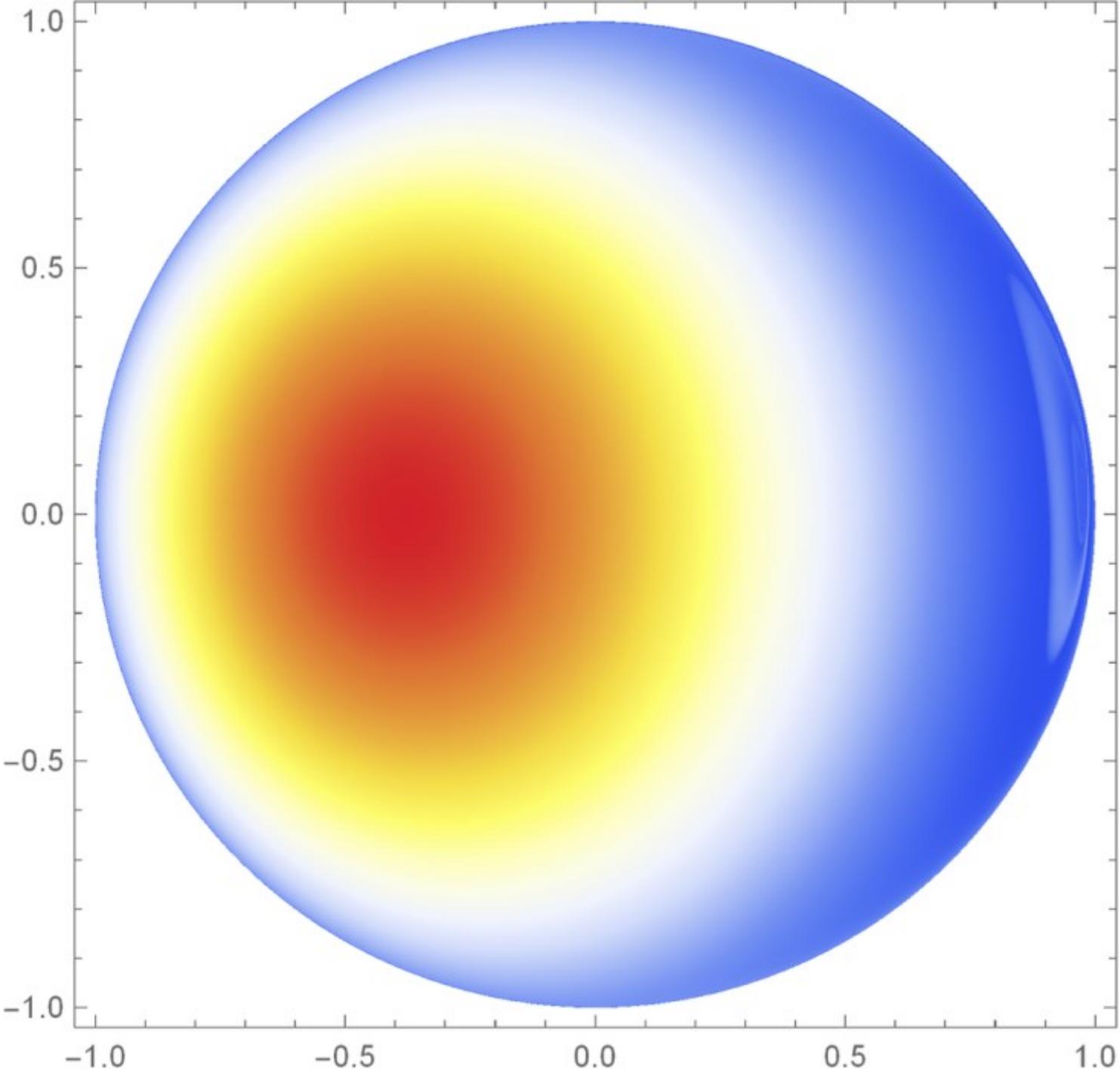
Visualization of the sheath collision operator

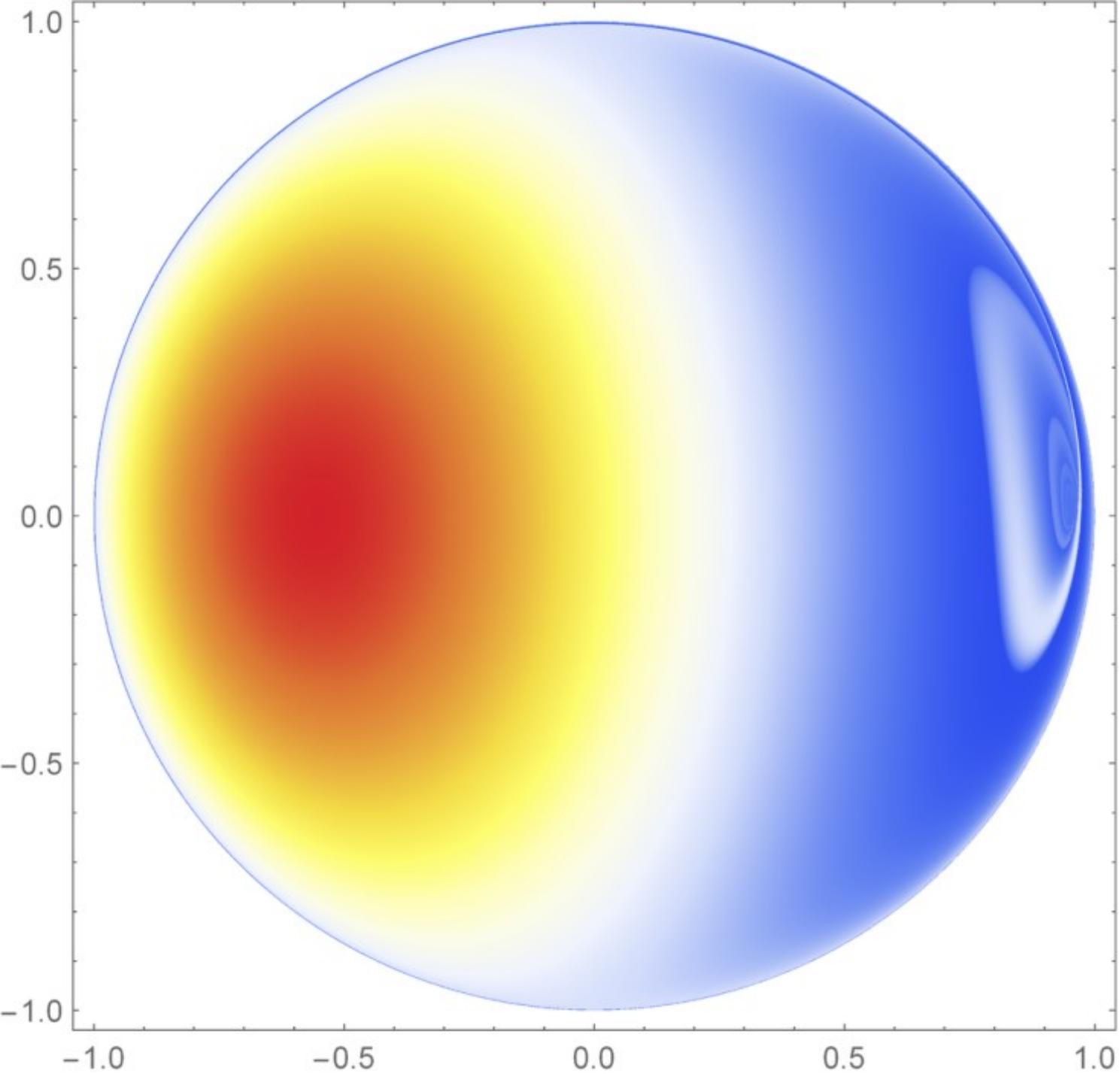


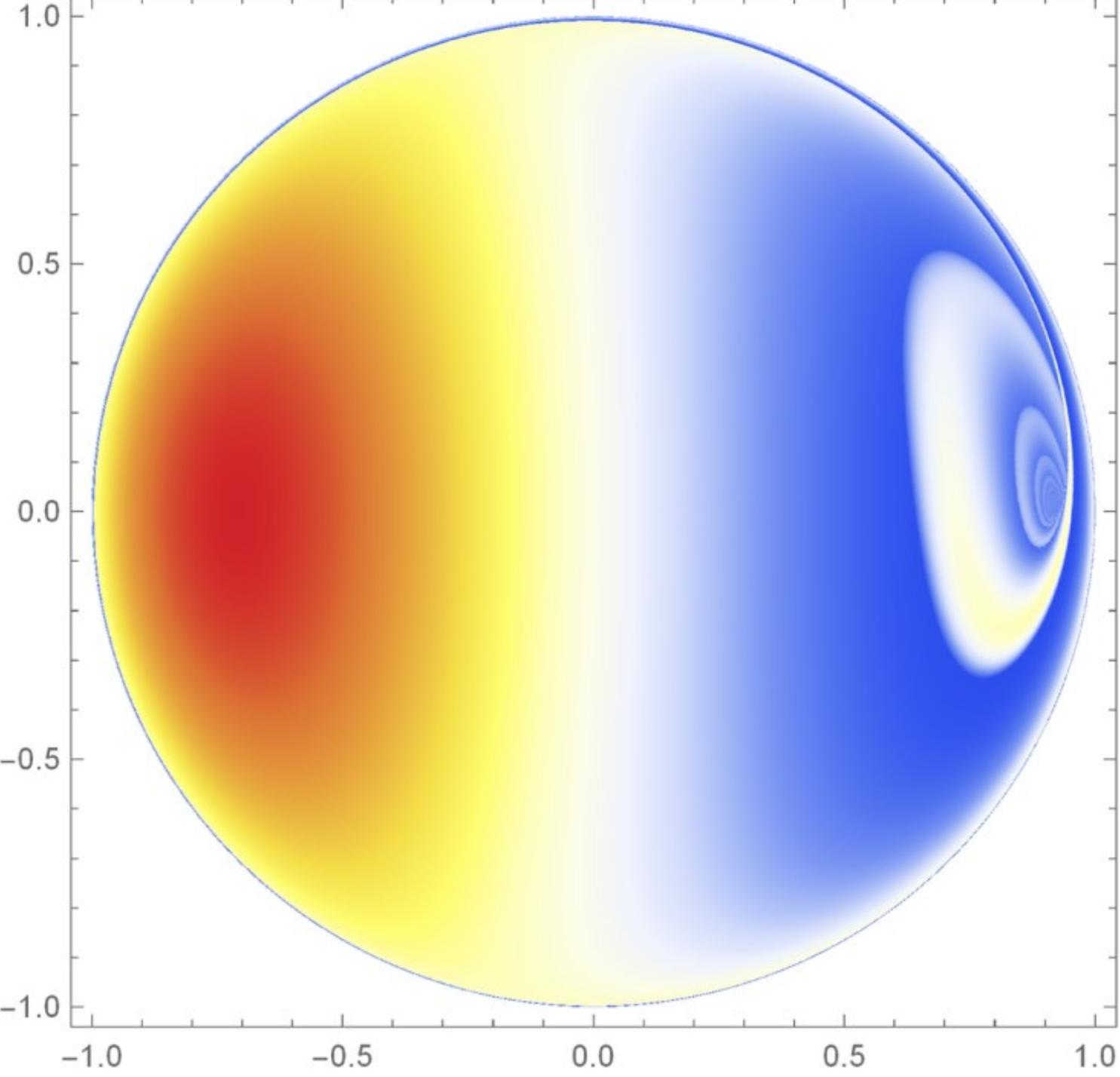
A gyro-invariant distribution is mapped to one with gyro structure.

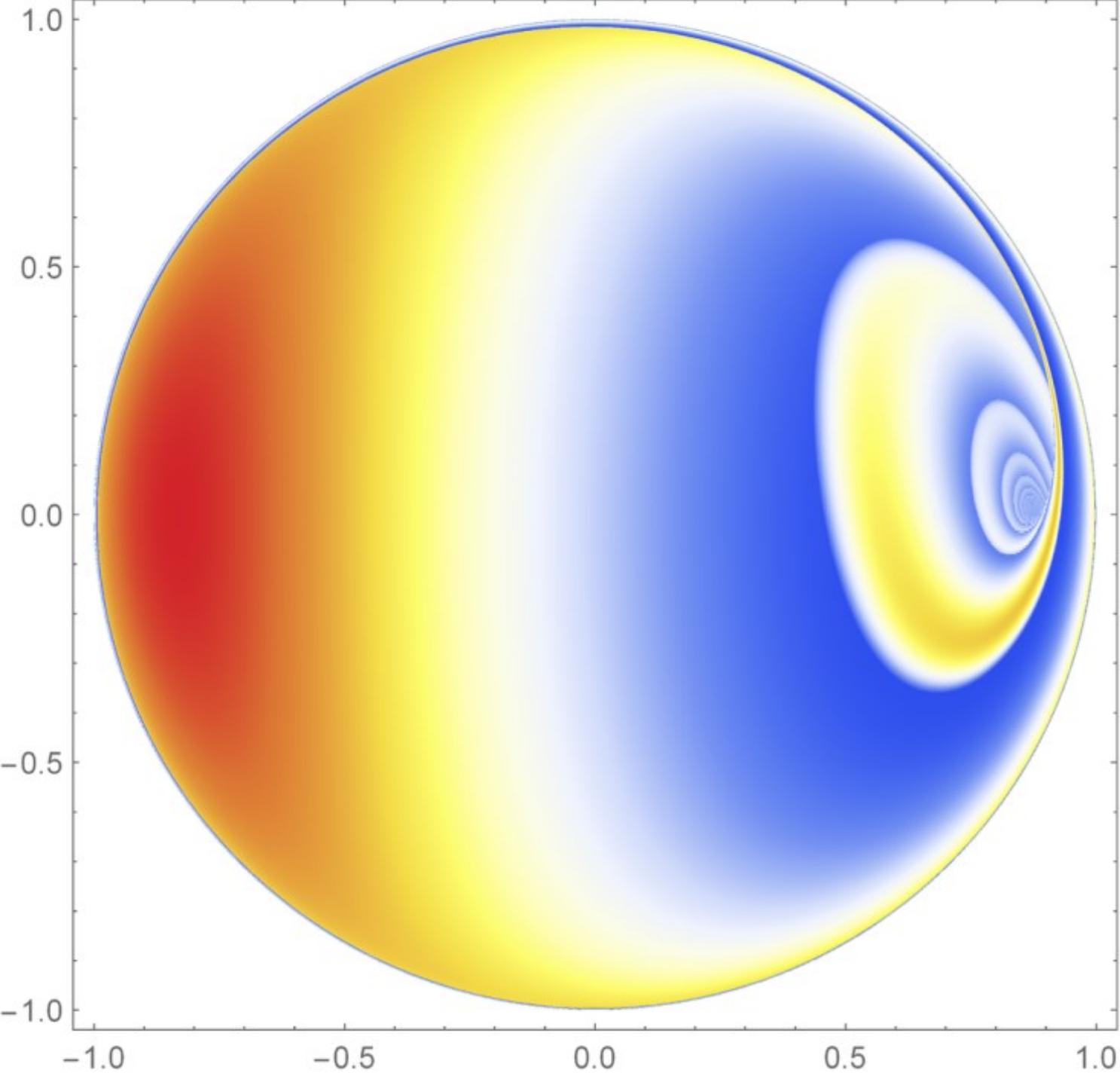


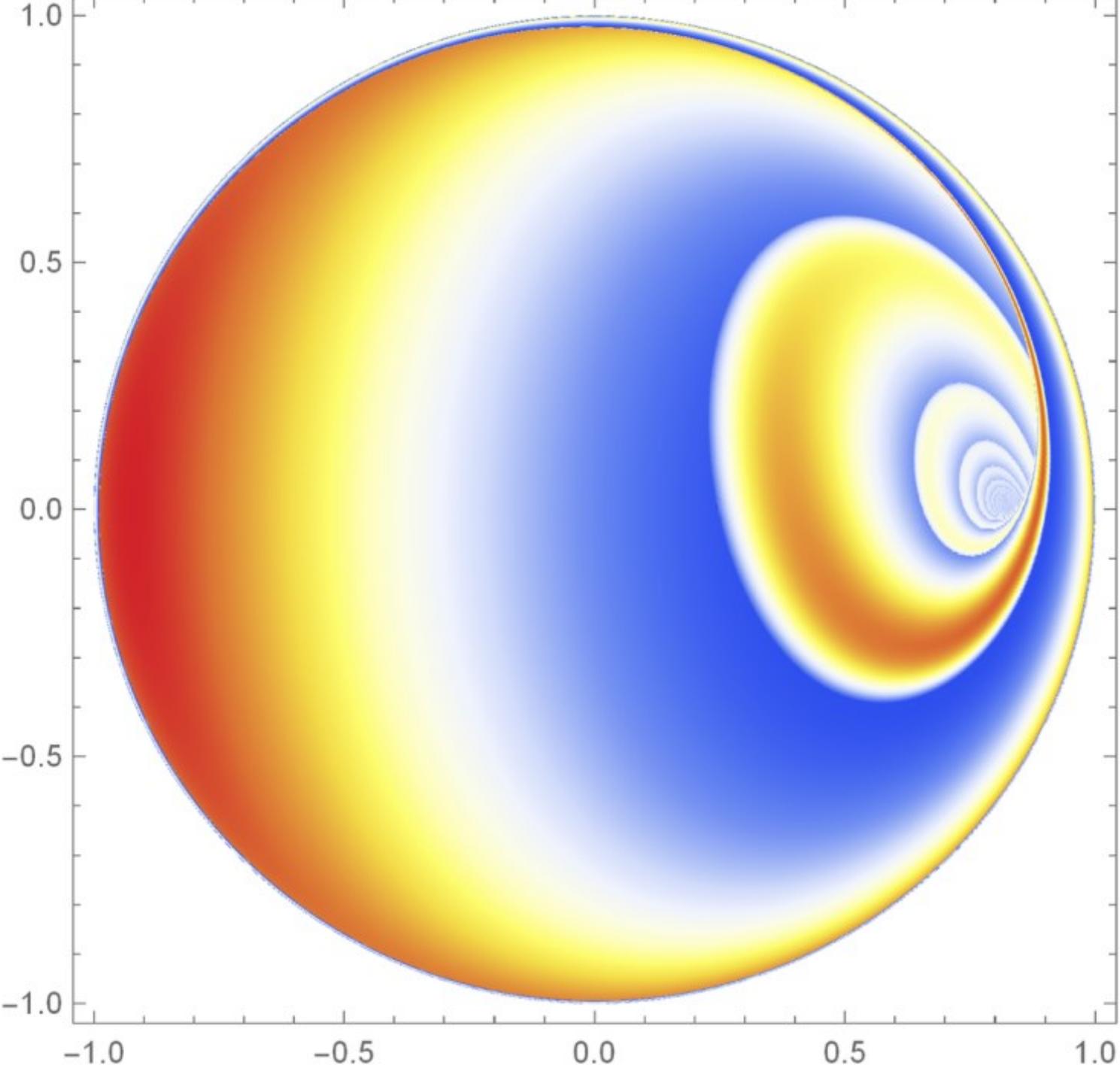


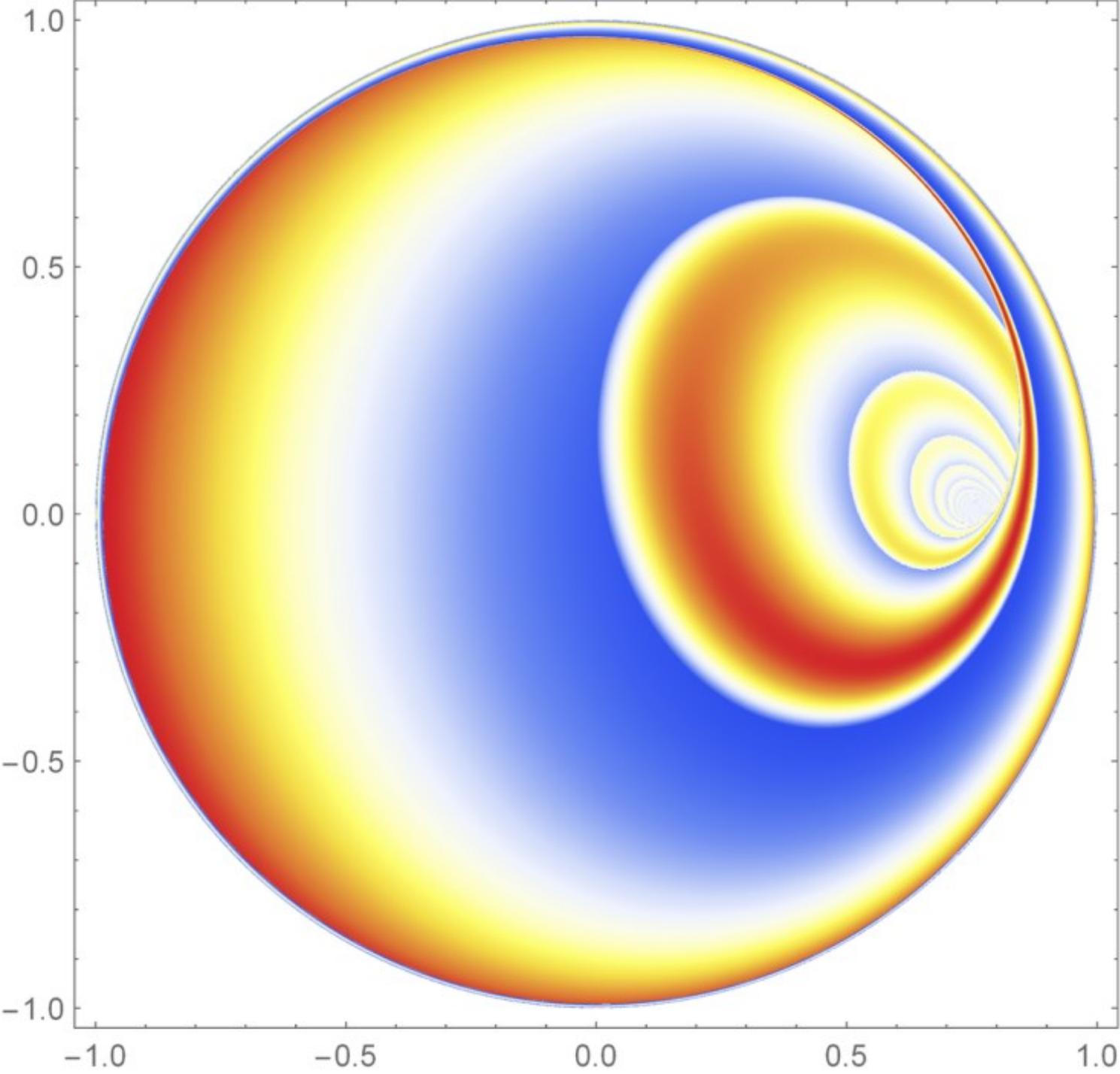


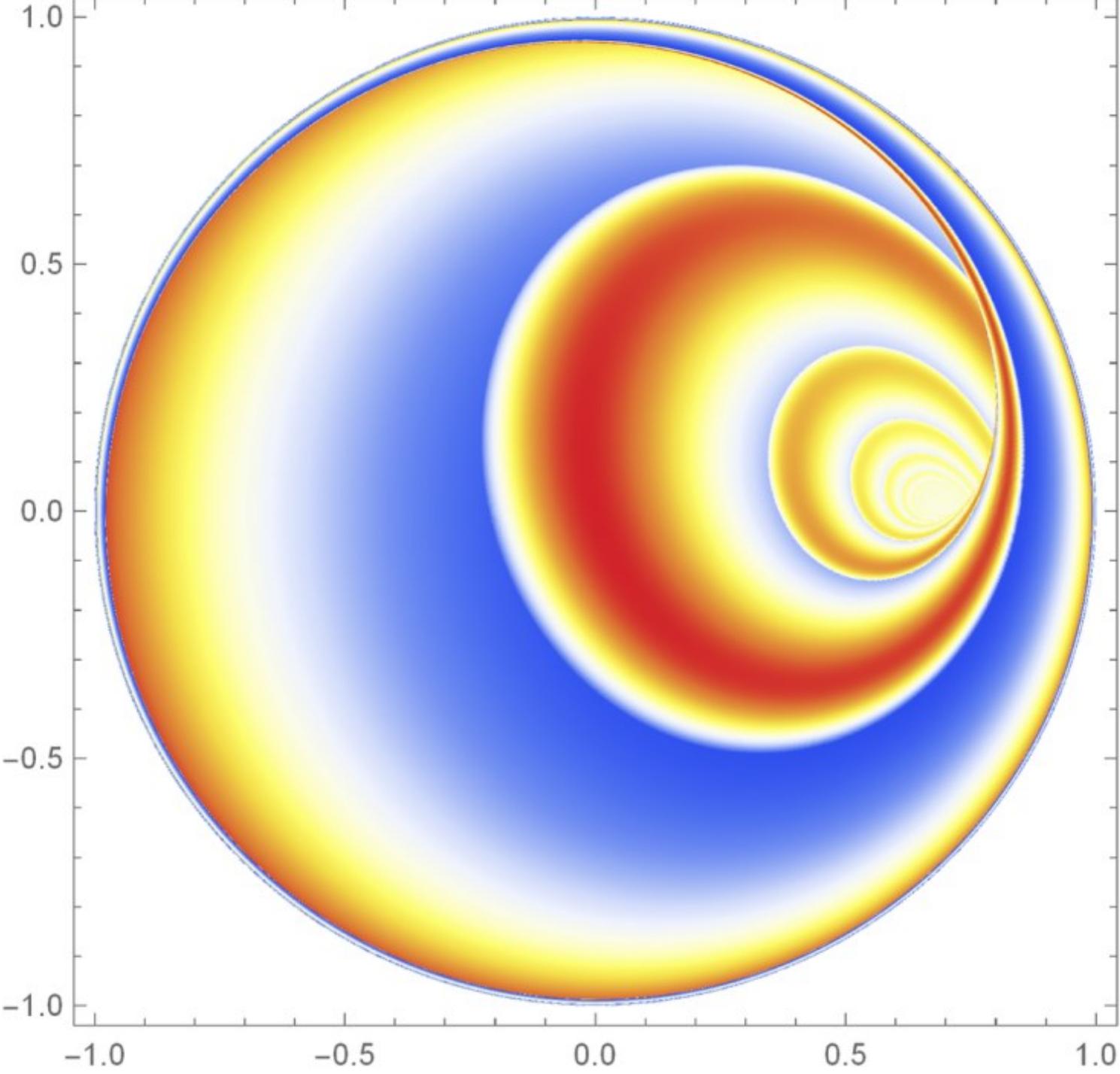


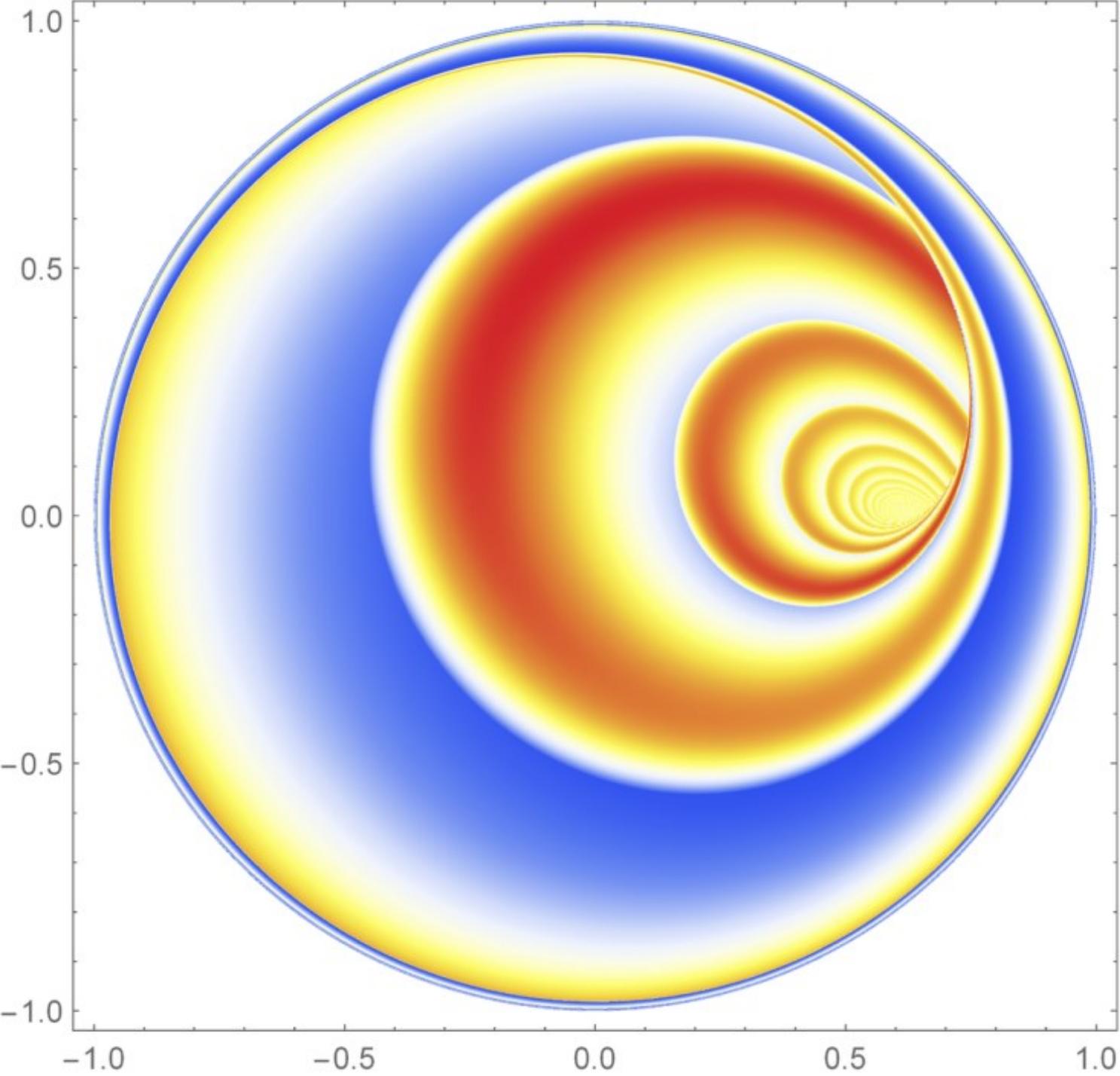


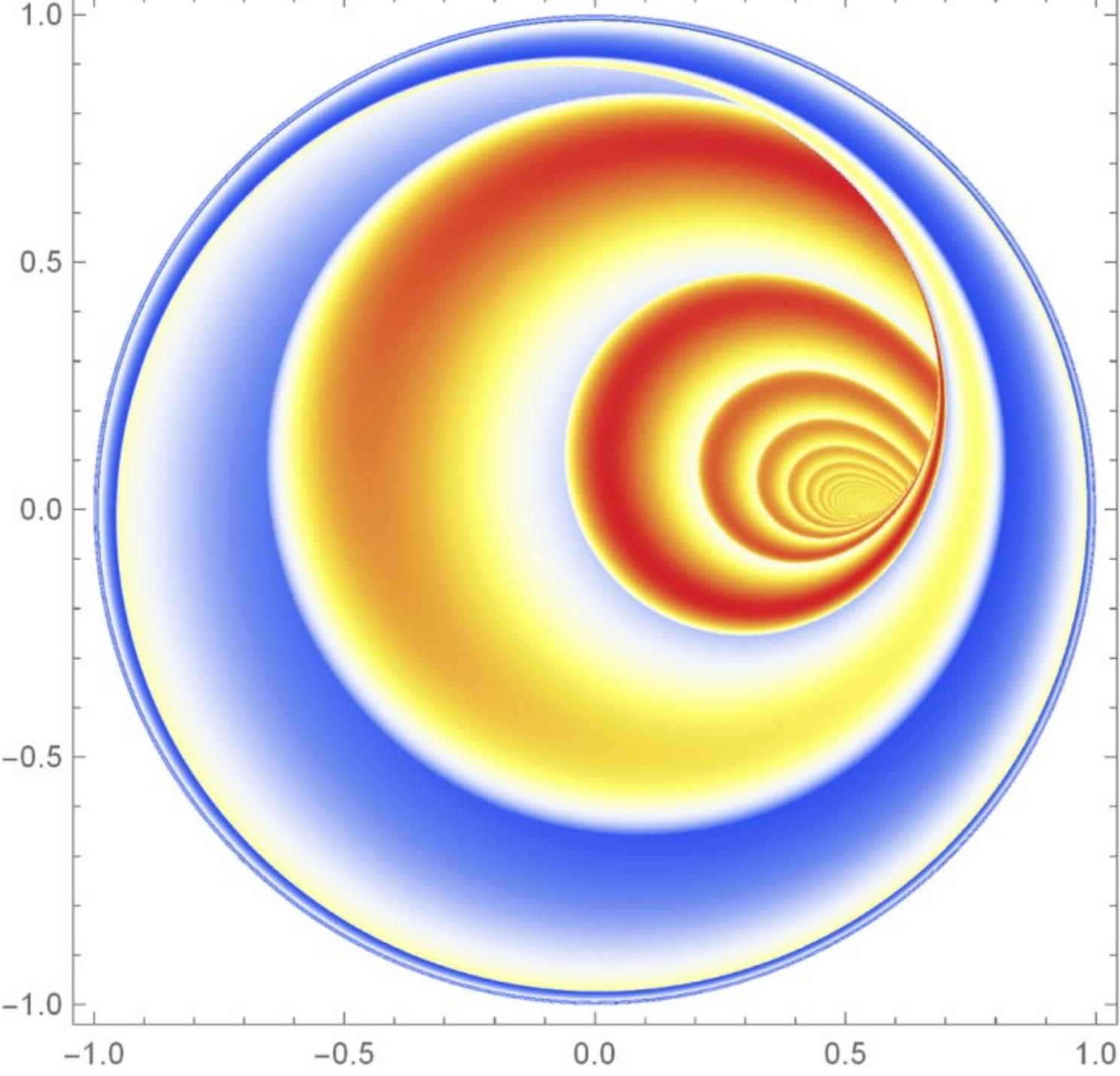


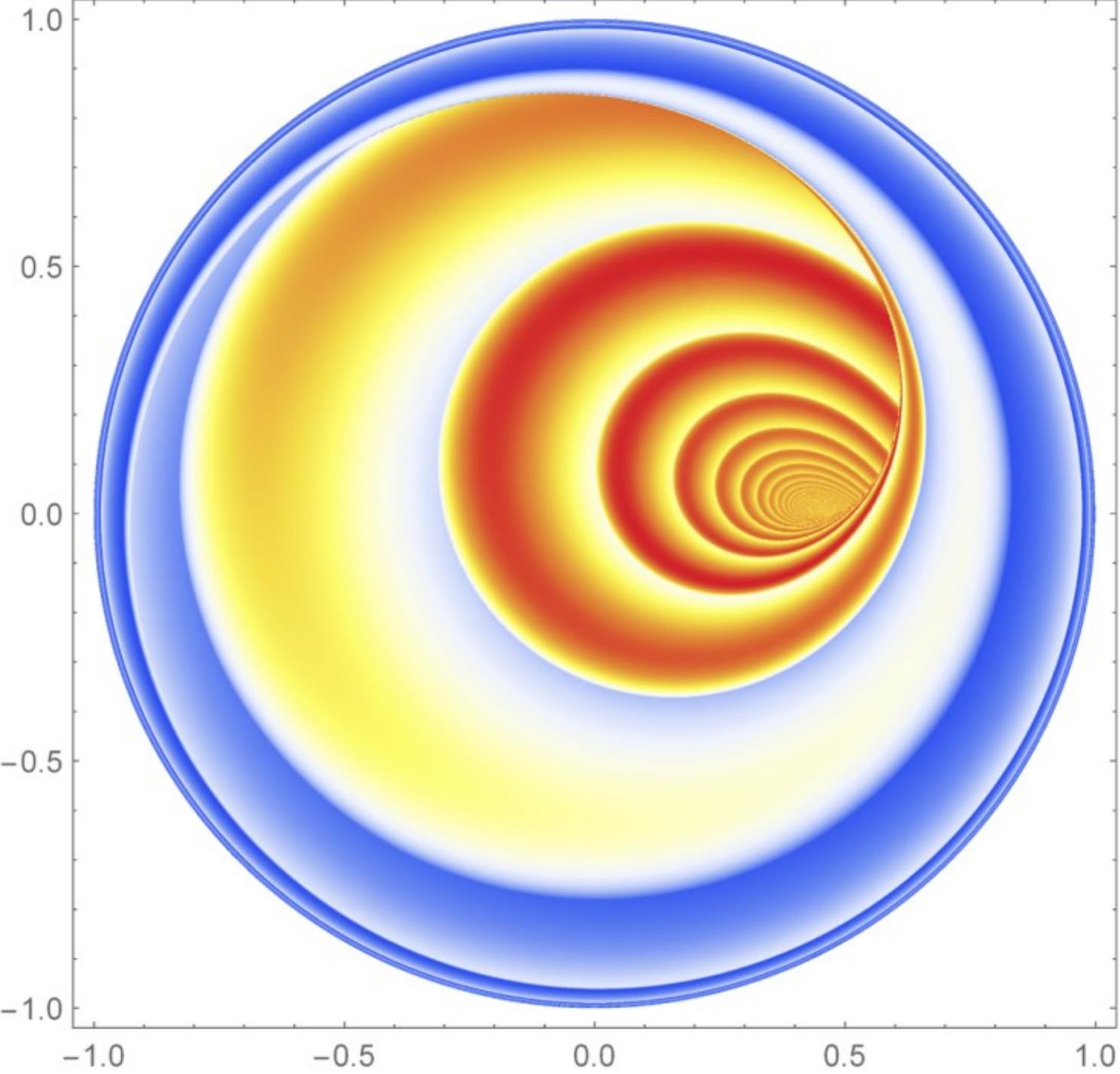


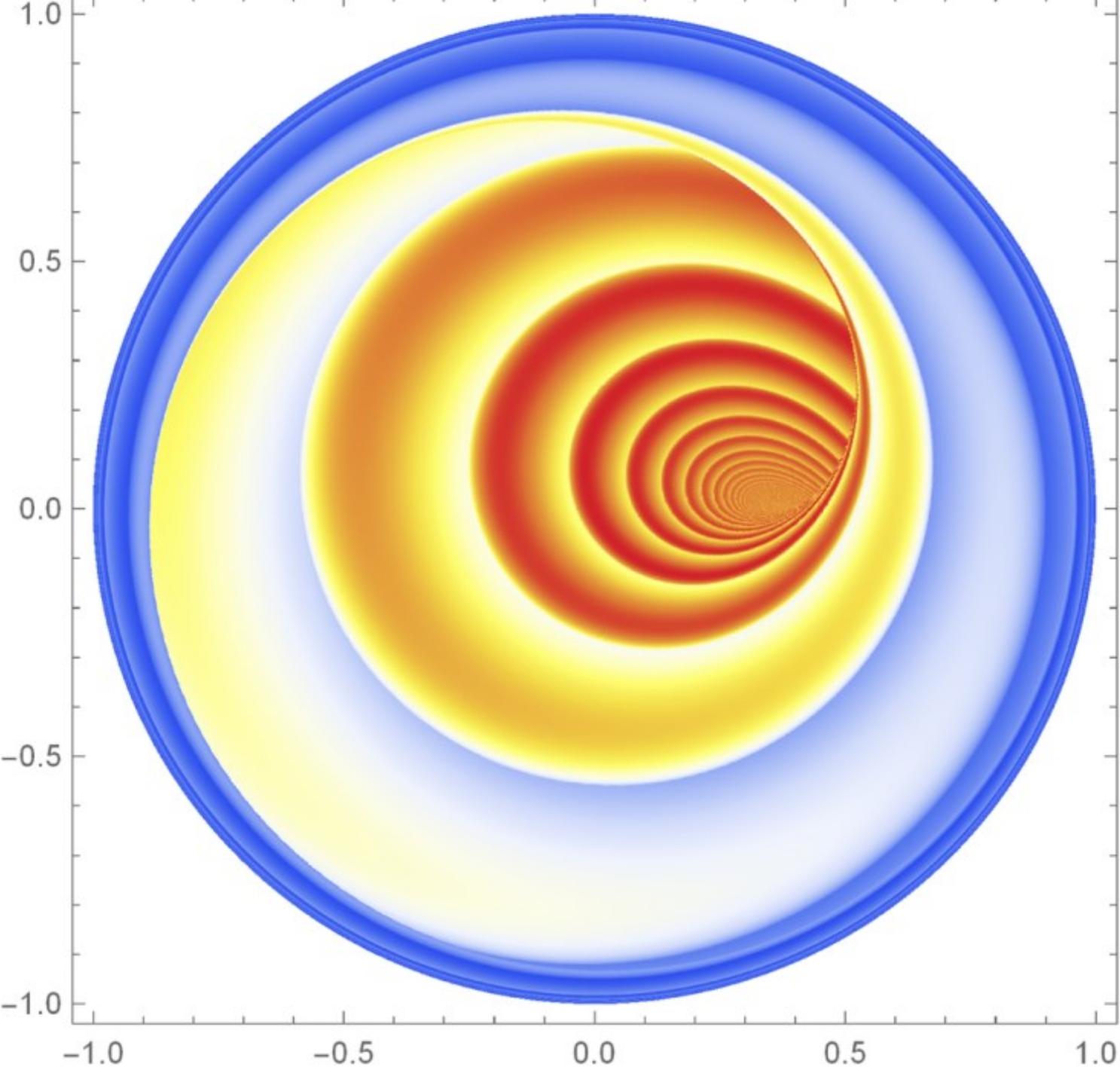


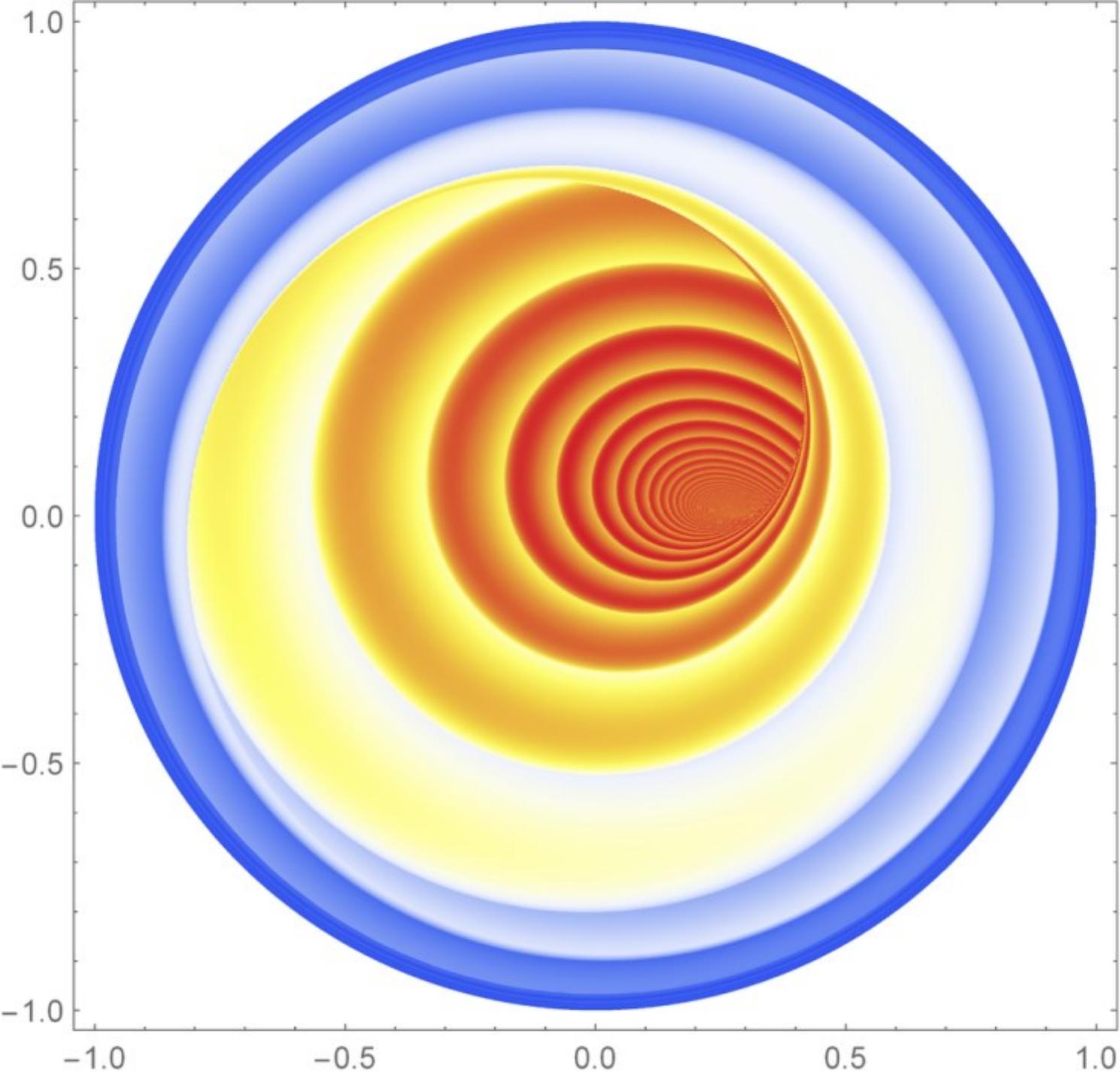


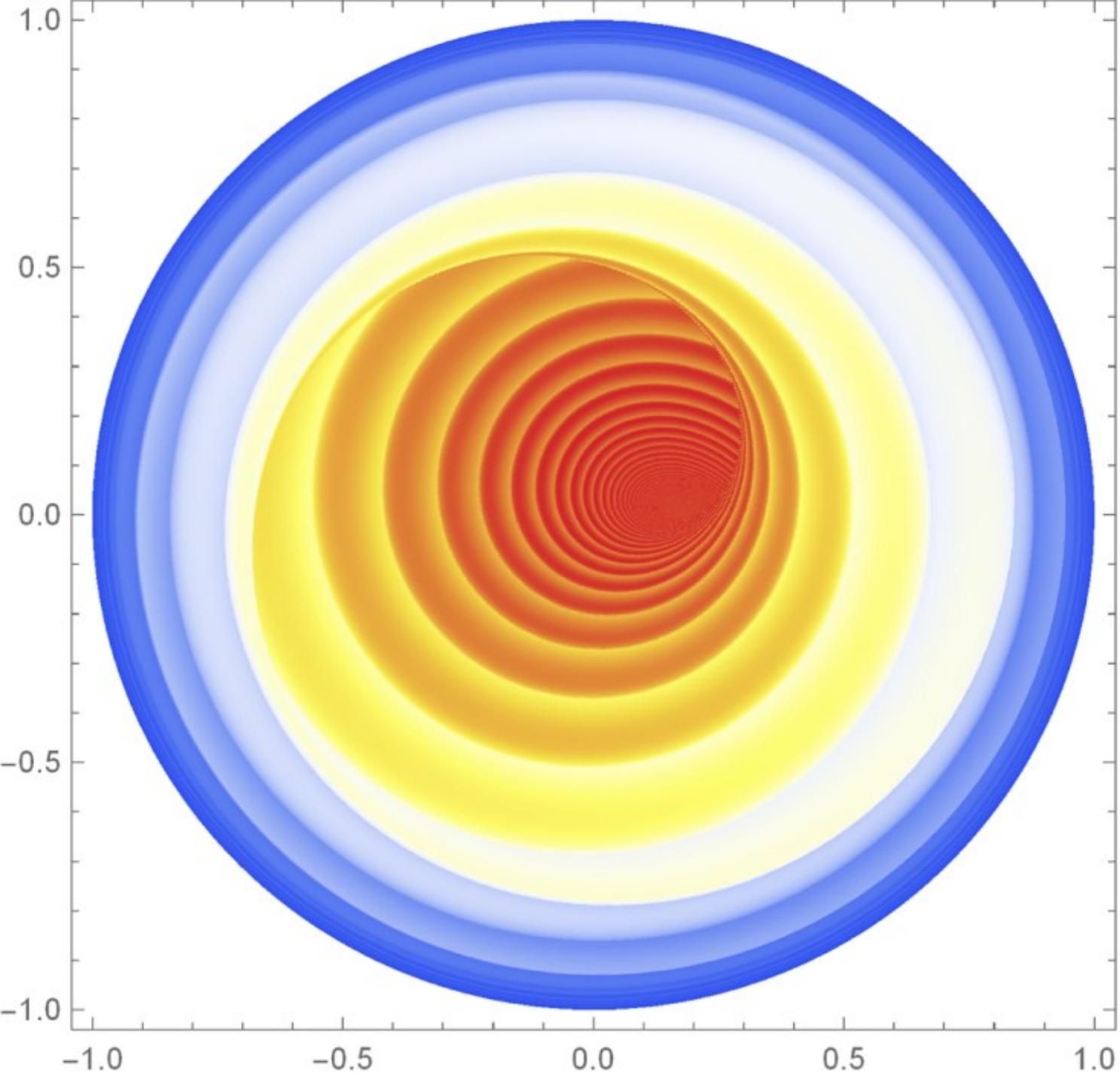


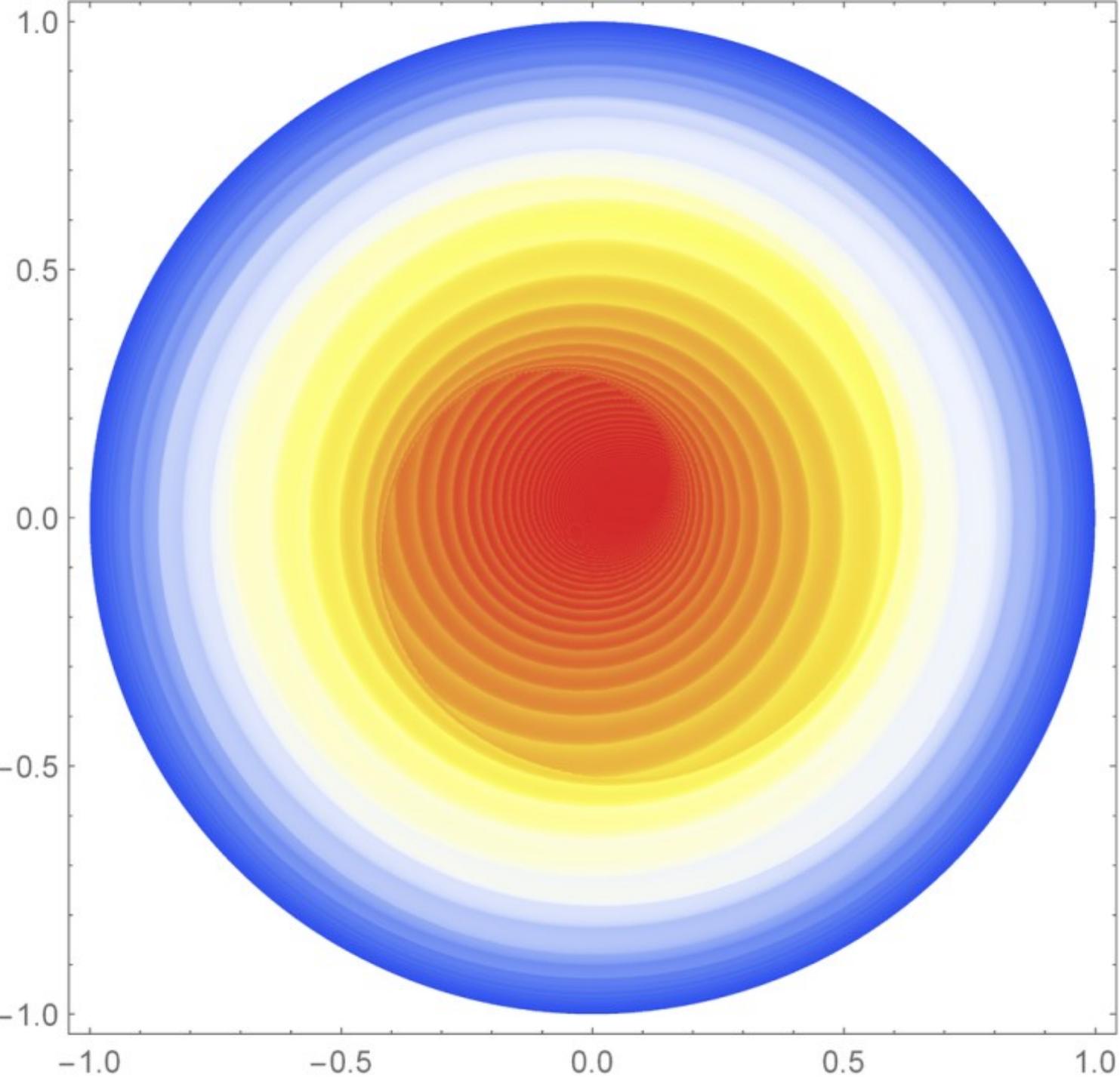


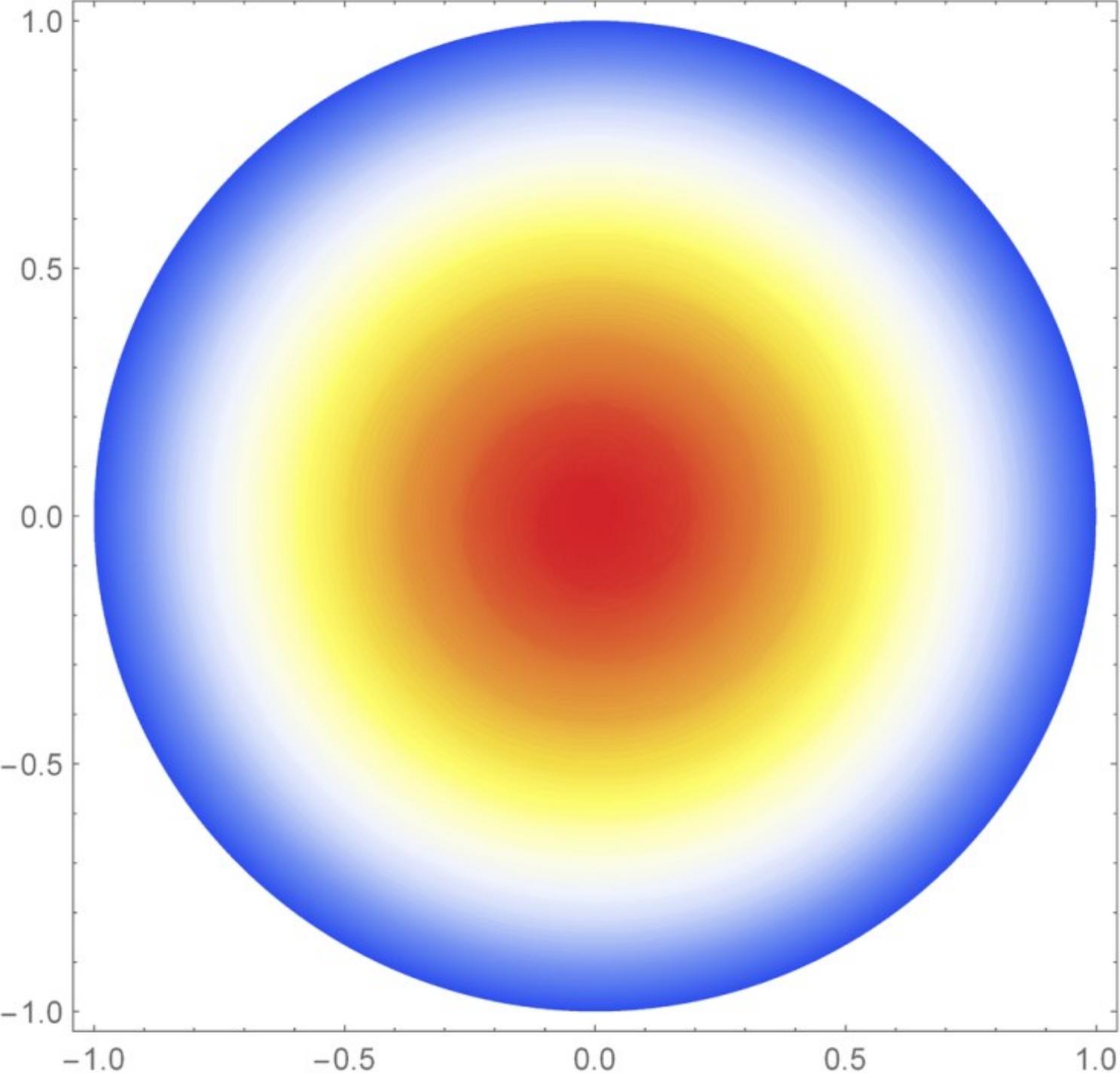




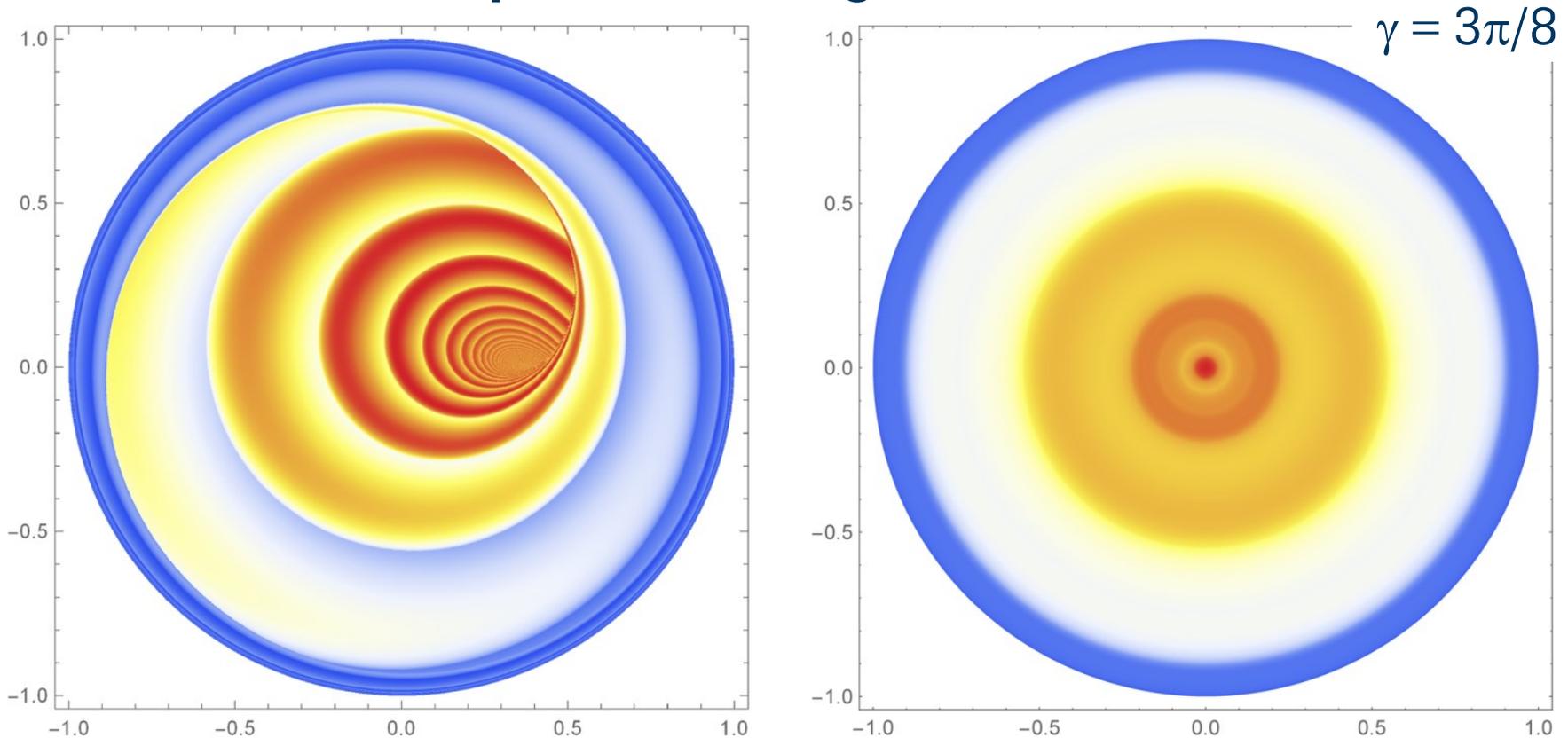






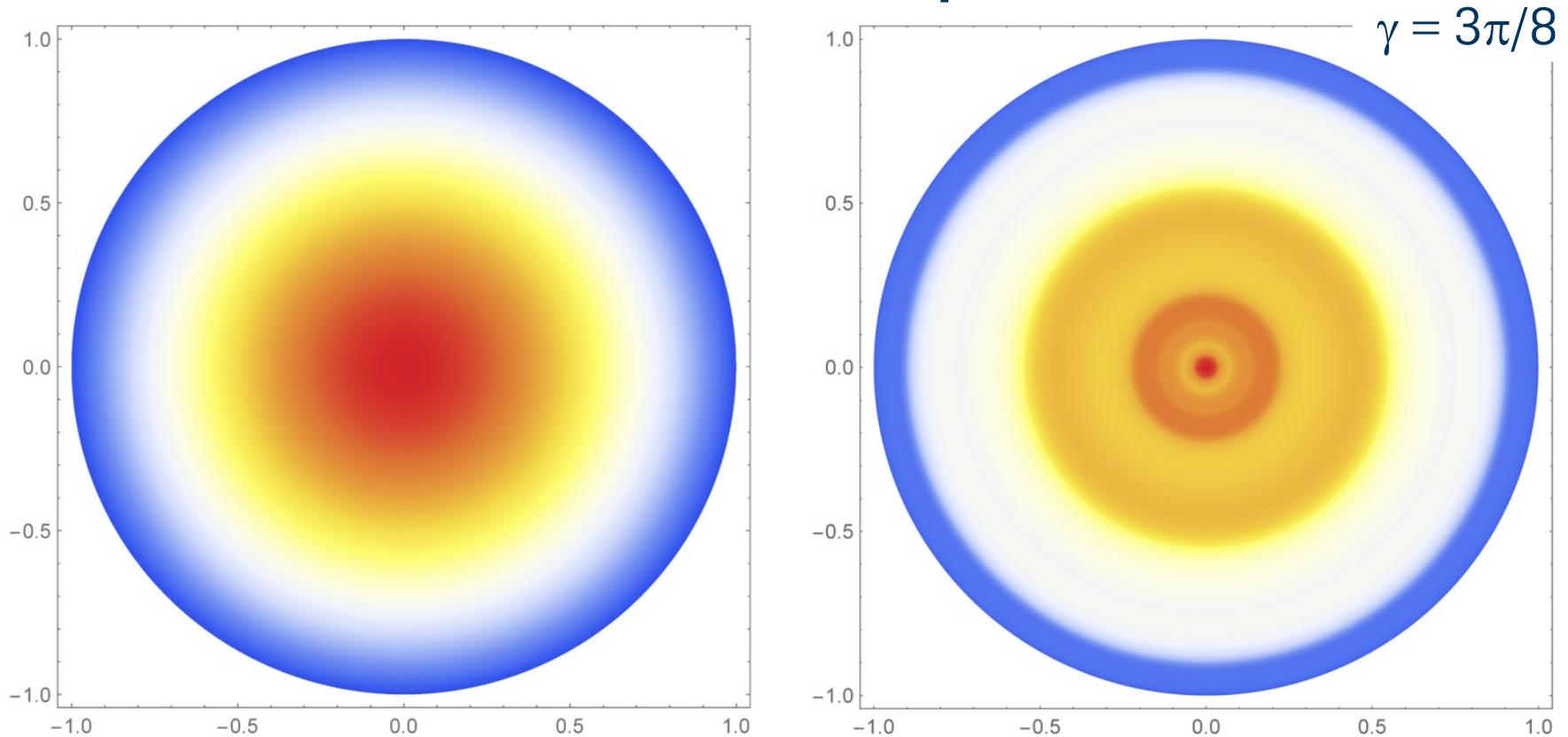


Visualization of phase mixing



A distribution with gyro structure is mapped to a gyro-invariant one.

Visualization of the combined operator



A gyro-invariant distribution is mapped to a gyro-invariant one.

Kinetic equation with new boundary conditions

In the local gyro coordinates, the kinetic equation reads:

$$\frac{\partial f}{\partial t} + \sqrt{2\epsilon} \cos \chi \frac{\partial f}{\partial s} - \Omega \frac{\partial f}{\partial \phi} = 0$$

Conditions at $s=0$ resulting from reflection and phase mixing:

$$f^{(\text{out})}(\epsilon, \chi) = \bar{T} f^{(\text{in})}(\epsilon, \chi) := \frac{1}{2\pi} \int_0^{2\pi} T f^{(\text{in})}(\epsilon, \chi) d\phi$$

The combined operator \bar{T} has a number of special properties:

- Particle flux and energy flux are conserved
- Free energy flux can be dissipated (but not generated)
- Incoming isotropic distributions yield isotropic outgoing ones
- Incoming gyro-invariant distributions yield gyro-invariant ones

Kinetic model on the global scale

Kinetic model on the global scale

Global scale kinetic equation, with explicit smallness parameter:

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \vec{r}} + \left(\vec{E} + \frac{1}{\delta} \vec{v} \times \vec{B} \right) \cdot \frac{\partial f}{\partial \vec{v}} = \langle f \rangle$$

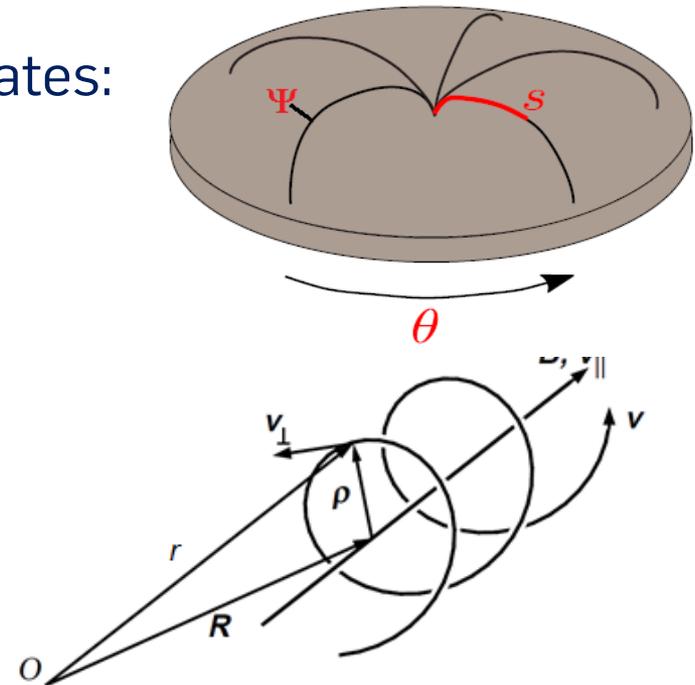
Transformation into global gyro coordinates:

$$\vec{R} = \vec{r} + \delta \frac{1}{B(\vec{r})} \vec{v} \times \vec{b}(\vec{r})$$

$$\epsilon = \frac{1}{2} \vec{v}^2$$

$$\chi = \arccos \left(\vec{v} \cdot \vec{b}(\vec{r}) / \sqrt{\vec{v}^2} \right)$$

$$\phi = \arctan \left(\vec{v} \cdot \vec{t}_2(\vec{r}) / \vec{v} \cdot \vec{t}_1(\vec{r}) \right)$$



Four time-scale formalism

Splitting the time into four independent time variables:

$$\frac{\partial}{\partial t} \rightarrow \sum_{k=-1} \delta^k \frac{\partial}{\partial t_k} = \frac{1}{\delta} \frac{\partial}{\partial t_{-1}} + \frac{\partial}{\partial t_0} + \delta \frac{\partial}{\partial t_1} + \delta^2 \frac{\partial}{\partial t_2} .$$

Ansatz of a formal series

$$f = f^{(0)} + \delta f^{(1)} + \delta^2 f^{(2)} + \delta^3 f^{(3)} + \dots$$

Substituting into the kinetic equation and sorting by powers of δ yields a system of (increasingly complex) differential equations:

$$EQ = \frac{1}{\delta} EQ_{-1} + EQ_0 + \delta EQ_1 + \delta^2 EQ_2 + \dots$$

► Idea: Average over fast time scales t_{-1} , t_0 , retain slow scale $t_1 + \delta t_2$

Four equations EQ₋₁, EQ₀, EQ₁, EQ₂

$$R\sqrt{2\epsilon} \sin \chi \frac{\partial f^{(0)}}{\partial t_{-1}} + L^{(-1)} f^{(0)} = 0$$

Simple

$$R\sqrt{2\epsilon} \sin \chi \frac{\partial f^{(1)}}{\partial t_{-1}} + L^{(-1)} f^{(1)} + L^{(0)} f^{(0)} + R\sqrt{2\epsilon} \sin \chi \frac{\partial f^{(0)}}{\partial t_0} + 2R\epsilon \sin^2 \chi \underline{J}_{s1}^{(1)} \sin \phi \frac{\partial f^{(0)}}{\partial t_{-1}} = \langle f \rangle^{(0)}$$

Relatively simple

$$\begin{aligned} R\sqrt{2\epsilon} \sin \chi \frac{\partial f^{(2)}}{\partial t_{-1}} + L^{(-1)} f^{(2)} + R\sqrt{2\epsilon} \sin \chi \frac{\partial f^{(1)}}{\partial t_0} + 2R\epsilon \sin^2 \chi \sin \phi \underline{J}_{s1}^{(1)} \frac{\partial f^{(1)}}{\partial t_{-1}} \\ + L^{(0)} f^{(1)} + R\sqrt{2\epsilon} \sin \chi \frac{\partial f^{(0)}}{\partial t_1} + 2R\epsilon \sin^2 \chi \sin \phi \underline{J}_{s1}^{(1)} \frac{\partial f^{(0)}}{\partial t_0} \\ + R(2\epsilon)^{3/2} \sin^3 \chi \left(\underline{J}^{(2)} + \underline{J}_{c2}^{(2)} \cos 2\phi \right) \frac{\partial f^{(0)}}{\partial t_{-1}} + L^{(1)} f^{(0)} = \langle f \rangle^{(1)} \end{aligned}$$

Complicated

$$\begin{aligned} R\sqrt{2\epsilon} \sin \chi \frac{\partial f^{(3)}}{\partial t_{-1}} + L^{(-1)} f^{(3)} + R\sqrt{2\epsilon} \sin \chi \frac{\partial f^{(2)}}{\partial t_0} + R2\epsilon \sin^2 \chi \underline{J}_{s1}^{(1)} \sin \phi \frac{\partial f^{(2)}}{\partial t_{-1}} + L^{(0)} f^{(2)} \\ + R\sqrt{2\epsilon} \sin \chi \frac{\partial f^{(1)}}{\partial t_1} + R2\epsilon \sin^2 \chi \underline{J}_{s1}^{(1)} \sin \phi \frac{\partial f^{(1)}}{\partial t_0} + R(2\epsilon)^{3/2} \sin^3 \chi \left(\underline{J}^{(2)} + \underline{J}_{c2}^{(2)} \cos 2\phi \right) \frac{\partial f^{(1)}}{\partial t_{-1}} + L^{(1)} f^{(1)} \\ + R\sqrt{2\epsilon} \sin \chi \frac{\partial f^{(0)}}{\partial t_2} + R2\epsilon \sin^2 \chi \underline{J}_{s1}^{(1)} \sin \phi \frac{\partial f^{(0)}}{\partial t_1} + R(2\epsilon)^{3/2} \sin^3 \chi \left(\underline{J}^{(2)} + \underline{J}_{c2}^{(2)} \cos 2\phi \right) \frac{\partial f^{(0)}}{\partial t_0} \\ + R(2\epsilon)^2 \sin^4 \chi \left(\underline{J}_{s1}^{(3)} \sin \phi + \underline{J}_{s3}^{(3)} \sin 3\phi \right) \frac{\partial f^{(0)}}{\partial t_{-1}} + L^{(2)} f^{(0)} = \langle f \rangle^{(2)} \end{aligned}$$

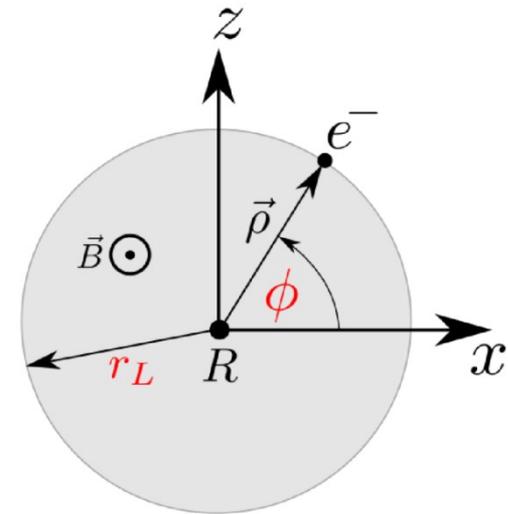
Very complicated

Equation EQ₋₁: Gyro motion around guiding center

Equation EQ₋₁ describes the gyro motion on the fast time scale t_{-1} :

$$\frac{\partial f^{(0)}}{\partial t_{-1}} - B \frac{\partial f^{(0)}}{\partial \phi} = 0$$

Under the assumption of gyro phase invariance, independence of $f^{(0)}$ on time t_{-1} and gyro phase ϕ



➔ Distribution function $f^{(0)}$ can be simplified

$$f^{(0)} = f^{(0)}(R, \Theta, Z, \epsilon, \chi, \phi, t_{-1}, t_0, t_1, t_2)$$

➔ Distribution functions $f^{(1)}$ and $f^{(2)}$ can be simplified

➔ Distribution function $f^{(3)}$ can be “integrated out”

Equation EQ₀: Bounce motion on a field line

Equation EQ₀ describes the bouncing motion on the time scale t_0 :

$$\frac{\partial f^{(0)}}{\partial t_0} + \sqrt{2\epsilon} \cos \chi \frac{\partial f^{(0)}}{\partial s} - \sqrt{2\epsilon} \cos \chi \frac{\partial \Phi}{\partial s} \frac{\partial f^{(0)}}{\partial \epsilon} + \sin \chi \left(\frac{1}{\sqrt{2\epsilon}} \frac{\partial \Phi}{\partial s} + \sqrt{\frac{\epsilon}{2}} \frac{1}{B} \frac{\partial B}{\partial s} \right) \frac{\partial f^{(0)}}{\partial \chi} = \langle f^{(0)} \rangle$$

➔ Distribution function $f^{(0)}$ in equilibrium on the field line:

$$f^{(0)} = \frac{n_i(\Psi, \Theta, s)}{(2\pi T_e(\Psi, \Theta))^{3/2}} \exp\left(-\frac{\epsilon}{T_e(\Psi, \Theta)}\right)$$

$$\Phi = V(\Psi, \Theta) - T_e(\Psi, \Theta) \ln(n_i(\Psi, \Theta, s))$$

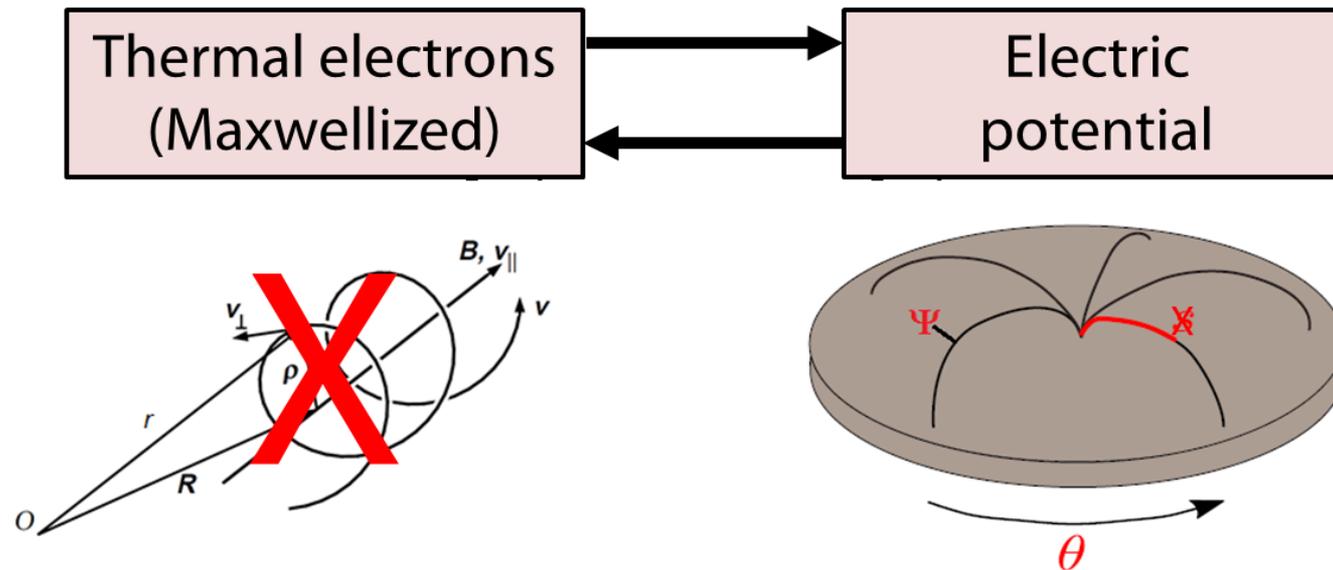
➔ Further information on distribution $f^{(1)}$; $f^{(2)}$ can be integrated out.

Equations EQ₁ and EQ₂ require some hard work



Reduced equations for $T_e(\Psi, \Theta)$ and $V(\Psi, \Theta)$

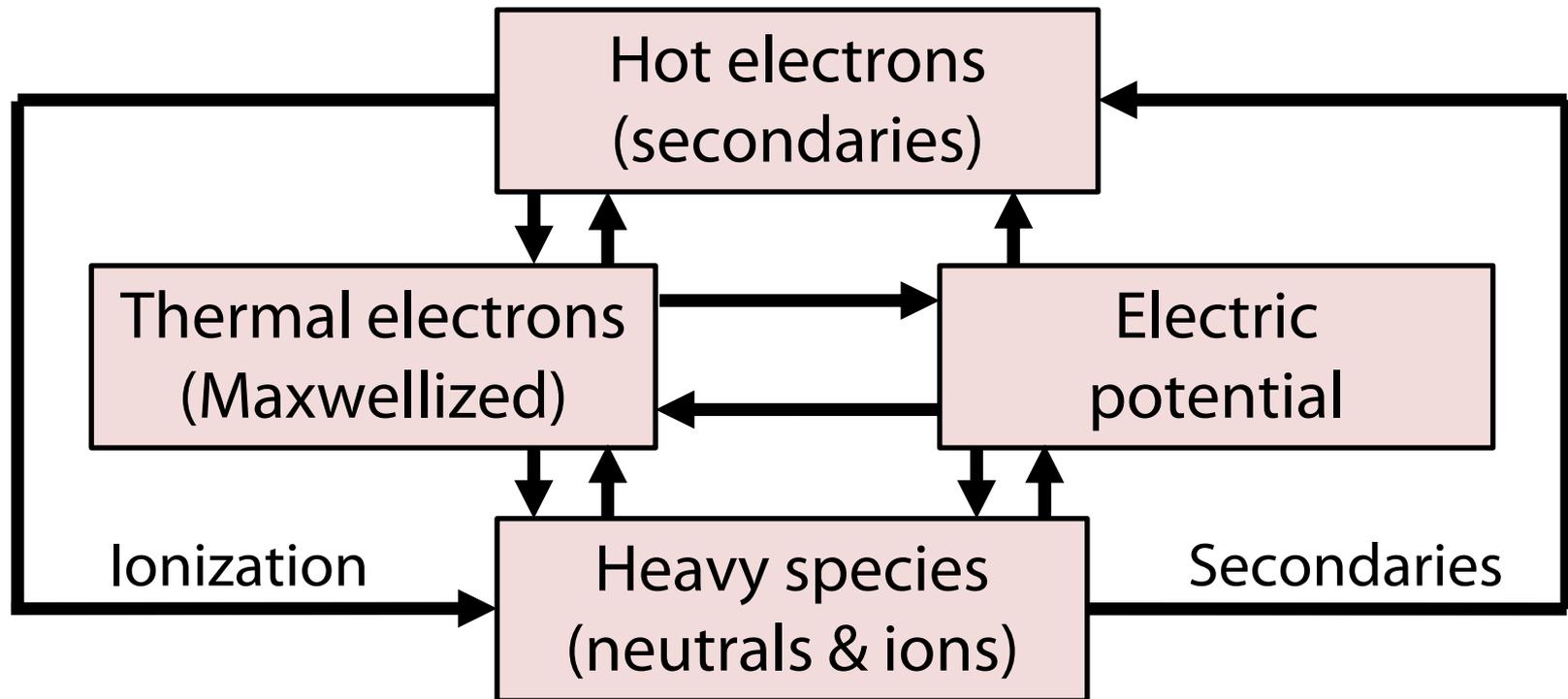
Equation EQ₁ and EQ₂ allow to derive a system of coupled parabolic differential equations for the field line parameters T_e and V in the spatial variables Ψ and Θ and in the combined time $t = t_1 + \delta t_2$:



Simplified, stiffness eliminated, must still be solved numerically.

Self-consistent description of magnetized technological plasmas

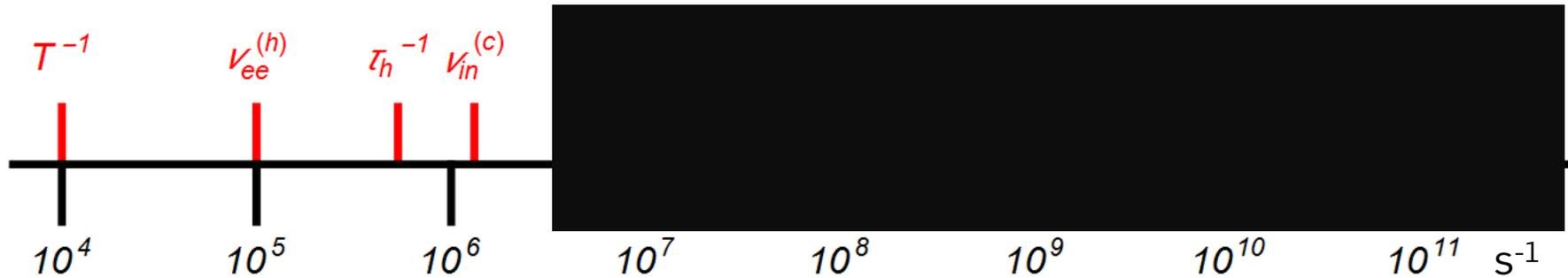
Integrating the other parts of the model



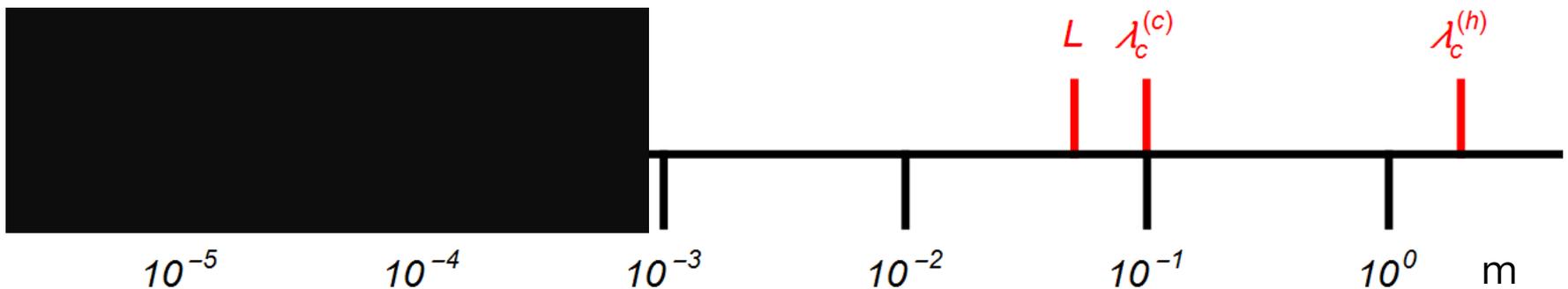
Self-consistent description of magnetized technological plasmas

What have we gained?

Characteristic times scales:



Characteristic length scales:



Reduction to two variables (Ψ , Θ), numerical stiffness eliminated!

Summary and outlook

Summary and outlook

Magnetized low pressure plasmas:

- Many technological applications (HIPIMS/PIAD/Thruster ...)
- Complicated physics, many different length and time scales
- Can only be treated by kinetic methods

Reduced kinetic theory exploits scaling $\lambda_D \ll s \ll r_L \ll \lambda \approx L$:

- Describes electron temperature and potential on field lines (ψ, Θ)
- Anomalous transport and Ohmic heating is covered
- Must still be numerically solved, but stiffness is eliminated

Future work: Self-consistent coupling to a model for ions/neutrals and to models for the target and the (possibly biased) substrate.

Thank you



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