Hydrodynamic manifolds for kinetic equations

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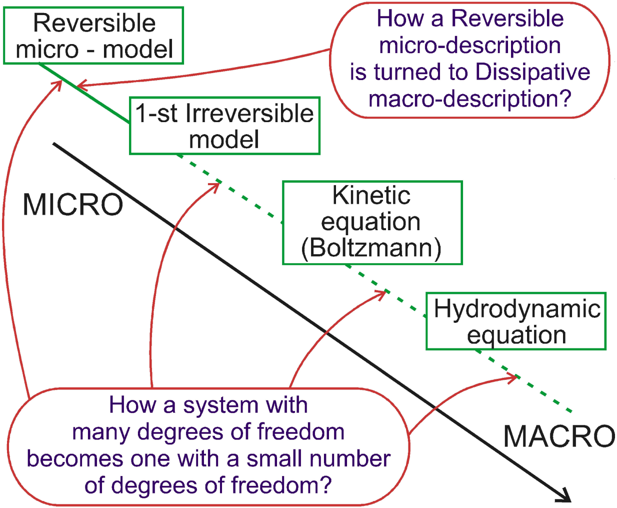
STEPS OF REDUCTION



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   - Navier–Stokes–Fourier equations
   - Van der Waals capillarity and Korteweg equations
   - Capillarity effects in ideal gas
2. From Boltzmann to Euler and Navier–Stokes–Fourier
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Fluid dynamics equations

Outline

Hydrodynamic fields

Consider the classical fluid, which is defined by the *hydrodynamic fields*: density ρ (scalar), velocity $\boldsymbol{u}$ (vector), and specific internal energy e, that is internal energy per unit of mass (scalar).
The everlasting conservation of mass

$$\boxed{\frac{\partial \rho}{\partial t} + \sum_j \frac{\partial(\rho u_j)}{\partial x_j} = 0.} \quad (1)$$

Caughy momentum equations

$$\boxed{\frac{\partial(\rho u_i)}{\partial t} + \sum_j \frac{\partial(\rho u_i u_j)}{\partial x_j} = \sum_j \frac{\partial \sigma_{ij}}{\partial x_j} + f_i.} \quad (2)$$

where $\boldsymbol{f} = (f_i)$ is the body force density, σ_{ii} ($i = 1, 2, 3$) are normal stresses, and σij ($i \neq j$) are shear stresses. The pressure p is

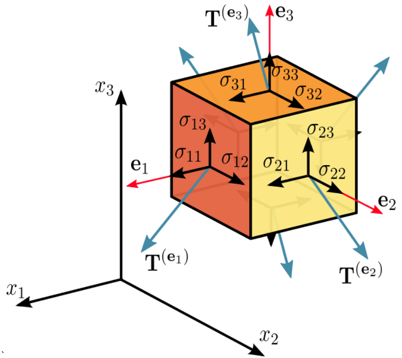
$$p = -\frac{1}{3}\mathrm{tr}\boldsymbol{\sigma} = -\frac{1}{3}\sum_i \sigma_{ii}$$

The Cauchy stress tensor $\boldsymbol{\sigma} = (\sigma_{ij})$ $(i,j = 1,2,3)$ describes the so-called *contact force*: Let for a small element of a body surface with area ΔS and outer normal vector $\boldsymbol{n} = (n_i)$ the stress tensor $\boldsymbol{\sigma}$ be given. Then the force applying *to the body* through this surface fragment is

$$\Delta \boldsymbol{F} = \boldsymbol{\sigma} \cdot \boldsymbol{n} \Delta S, \text{ that is, } F_i = \Delta S \sum_j \sigma_{ij} n_j.$$

The stress tensor is symmetric (to provide conservation of angular momentum), $\sigma_{ij} = \sigma_{ji}$.

Cauchi stress



$$\mathbf{T}^{(\mathbf{n})} = \mathbf{n} \cdot \boldsymbol{\sigma} \quad \text{or} \quad T_j^{(n)} = \sigma_{ij} n_i.$$

If the material body Ω experiences infinitisemal *displacement* $\boldsymbol{x} \mapsto \boldsymbol{x} + \delta \boldsymbol{r}(\boldsymbol{x})$, which vanishes with derivatives on the boundary, then the *work of the contact forces* is (use the Stokes formula for integration by parts):

$$\delta W = \int_{\Omega} \sum_{i,j} \frac{\partial \sigma_{ij}}{\partial x_j} \delta r_i \, d^3x = - \int_{\Omega} \sum_{i,j} \sigma_{ij} \frac{\partial \delta r_i}{\partial x_j} d^3x. \qquad (3)$$

Take into account symmetry of σ_{ij}:

$$\delta W = -\frac{1}{2} \int_{\Omega} \sum_{i,j} \sigma_{ij} \left(\frac{\partial \delta r_i}{\partial x_j} + \frac{\partial \delta r_j}{\partial x_i} \right) d^3x.$$

The *power produced by the contact forces* is

$$\boxed{P = -\frac{1}{2} \int_{\Omega} \sum_{i,j} \sigma_{ij} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) d^3x} \qquad (4)$$

The conservation of energy

$$\boxed{\frac{\partial(\rho\epsilon)}{\partial t}+\sum_j\frac{\partial(\rho\epsilon u_j)}{\partial x_j}=\sum_{ij}\sigma_{ij}\frac{\partial u_i}{\partial x_j}+\sum_i f_i u_i-\sum_i\frac{\partial q_i}{\partial x_i},} \quad (5)$$

where ϵ is the energy density per unit mass: $\epsilon = e + \frac{1}{2}u^2$,
e is the *specific internal energy*, $u^2 = \sum_i u_i^2$,
$\boldsymbol{q} = (q_i)$ is the vector of *heat flux* (thermal conductivity).

For the perfect (monoatomic) gas, $e = \frac{3R}{2M}\theta$, where R is the ideal gas constant, M is the molar mass and θ is the absolute temperature.

Outline

Navier–Stokes stress tensor and Fourier heat flux

How can we express the stress tensor and the heat flux through the hydrodynamic fields: density ρ, velocity $\boldsymbol{u}$, and specific internal energy e?

The simplest (*linear response*) answer is given by the Navier–Stokes stress tensor and Fourier heat flux:

$$\boxed{\begin{aligned} \sigma_{ij} &= \sigma_{ij}^{E} + \sigma_{ij}^{V};\\ \sigma_{ij}^{E} &= -p\delta_{ij};\\ \sigma_{ij}^{V} &= \lambda\delta_{ij}\sum_{k}\frac{\partial u_k}{\partial x_k} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right);\\ q_i &= -\kappa\frac{\partial \theta}{\partial x_i}. \end{aligned}} \tag{6}$$

Power produced by viscosity

The power produced by the Navier–Stokes viscous stress is

$$P = -\lambda \left(\sum_i \frac{\partial u_i}{\partial x_i} \right)^2 - \frac{\mu}{2} \sum_{ij} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)^2 .$$

If $\mu > 0$ and $3\lambda + 2\mu \geq 0$ then $P \leq 0$ (i.e. viscosity is friction, indeed).

Navier–Stokes–Fourier equations for ideal gas

$$\frac{\partial \rho}{\partial t} + \sum_j \frac{\partial(\rho u_j)}{\partial x_j} = 0;$$

$$\frac{\partial(\rho u_i)}{\partial t} + \sum_j \frac{\partial(\rho u_i u_j)}{\partial x_j} + \frac{R}{M}\frac{\partial(\rho\theta)}{\partial x_i}$$

$$= \frac{\partial}{\partial x_i}\left(\lambda \sum_k \frac{\partial u_k}{\partial x_k}\right) + \sum_j \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + f_i;$$

$$\frac{\partial(\rho[\frac{3R}{2M}\theta + \frac{1}{2}u^2])}{\partial t} + \sum_j \frac{\partial(\rho[\frac{3R}{2M}\theta + \frac{1}{2}u^2]u_j)}{\partial x_j} + \rho\theta\frac{R}{M}\sum_i \frac{\partial u_i}{\partial x_i}$$

$$= \lambda\left(\sum_i \frac{\partial u_i}{\partial x_i}\right)^2 + \frac{\mu}{2}\sum_{ij}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)^2 + \sum_i f_i u_i + \sum_i \frac{\partial}{\partial x_i}\left(\kappa \frac{\partial \theta}{\partial x_i}\right).$$

Outline

Timeline of capillarity

- In 1877, Gibbs published the theory of capillarity. He introduced and studied thermodynamics of two-dimensional objects – surfaces of discontinuity.
- In 1893, van der Waals proposed the theory of capillarity using the hypothesis that density of the body varies continuously and energy depends on the *gradient of density*.
- Van der Waals proposed to include in the energy density a new term, $(c\,\mathrm{grad}\rho)^2$, where ρ is density and c is the capillarity coefficient.
- In 1901, His doctorate student, Korteweg, found, how this term affects the motion of fluids, and created the dynamics of fluids with capillarity.

The van der Waals capillarity term plays essential role in many important achievements:

- In the Landau theory of phase transitions;
- In the Ginzburg–Landau theory of superfluids and superconductors;
- In the Cahn–Hilliard models of process of phase separation ($\rho_t = -a\Delta - b\Delta^2 +$ kinetic terms);
- In the Langer Bar-On and Miller theory of spinodal decomposition;
- In all modern ‘phase field’ models of multiphase systems.

Van der Waals energy

Represent the Gibbs free energy of a body Ω as a sum, $G = G_0 + G_K$,

$$\begin{aligned} G_0 &= \int_\Omega g_0(\rho,\theta)d^3x; \\ G_K &= \int_\Omega K(\rho,\theta)\sum_i \left(\frac{\partial\rho}{\partial x_i}\right)^2 d^3x \\ &= -\int_\Omega \rho \sum_i \frac{\partial}{\partial x_i}\left(K(\rho,\theta)\frac{\partial\rho}{\partial x_i}\right) d^3x \end{aligned} \tag{7}$$

Korteweg stress tensor

Korteweg found the corresponding to G_K addition to the stress tensor:

$$\sigma_{ij}^K = \rho\left[\sum_k \frac{\partial}{\partial x_k}\left(K(\rho,\theta)\frac{\partial \rho}{\partial x_k}\right)\right]\delta_{ij} - K(\rho,\theta)\frac{\partial \rho}{\partial x_i}\frac{\partial \rho}{\partial x_j} \quad (8)$$

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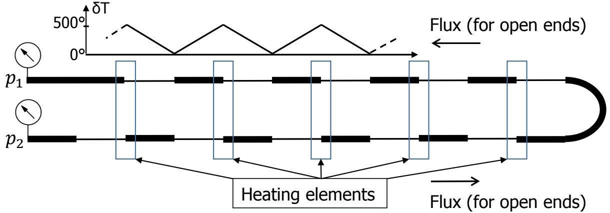
Light mill (Crookes radiometer)

Knudsen pump

p_1 (mmHg)	p_2 (mmHg)	p_1/p_2
760	760	1
235.1	235.0	1.0005
65.2	64.8	1.006
16.5	15.1	1.09
4.834	2.058	2.35
3.601	1.169	3.09
0.475	0.0476	9.98
0.278	0.0314	8.85
0.0978	0.00419	2.33



Model reduction and slow manifolds

Outline

2. From Boltzmann to Euler and Navier–Stokes–Fourier
   - Reduction problem
   - Two programs of the way "to the laws of motion of continua"

3. Invariance equation and Chapman–Enskog series
   - Invariance equation
   - The Chapman–Enskog expansion

From Boltzmann equation to fluid dynamics: Three main questions

Hilbert has specified a particular case of the 6th problem: From Boltzmann equation to fluid dynamics.
Three questions arise:

1. Is there hydrodynamics in the kinetic equation, i.e., is it possible to lift the hydrodynamic fields to the relevant one-particle distribution functions in such a way that the projection of the kinetics back satisfies some hydrodynamic equations?
2. Do these hydrodynamics have the conventional Euler and Navier–Stokes–Fourier form?
3. Do the solutions of the kinetic equation degenerate to the hydrodynamic regime (after some transient period)?

The Boltzmann equation

We discuss today two groups of examples.

1. Kinetic equations which describe the evolution of a one-particle gas distribution function $f(t, \boldsymbol{x}; \boldsymbol{v})$

$$\partial_t f + \boldsymbol{v} \cdot \nabla_x f = \frac{1}{\epsilon} Q(f),$$

   where $Q(f)$ is the collision operator.

2. The Grad moment equations produced from these kinetic equations.

McKean diagram (1965) (IM=Invariant Manifold)

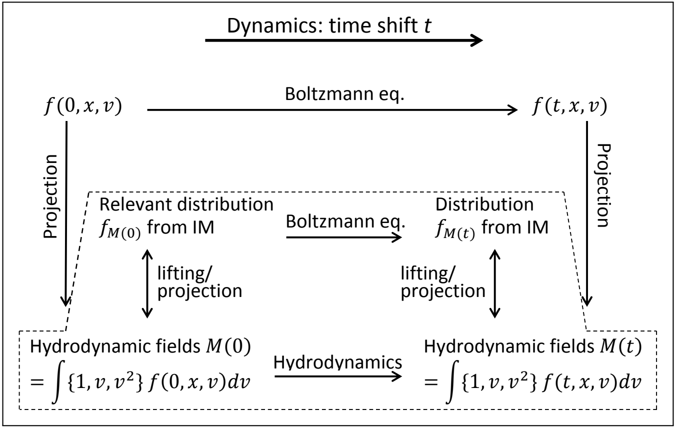
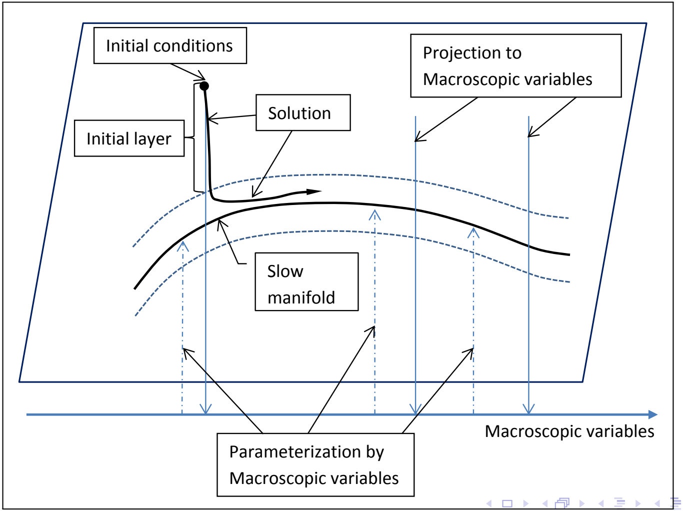


Figure: The diagram in the dashed polygon is commutative.

Singular perturbations and slow manifold diagram



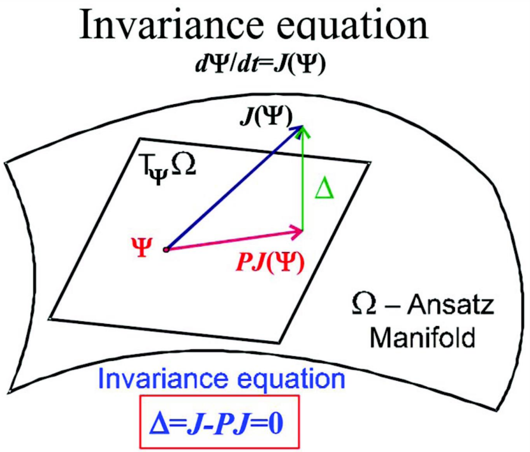
The doubt about small parameter (McKean, Slemrod)

- Introduce a new space-time scale, $x' = \epsilon^{-1}x$, and $t' = \epsilon^{-1}t$. The rescaled equations do not depend on ϵ at all and are, at the same time, equivalent to the original systems.
- The presence of the small parameter in the equations is virtual. “Putting ϵ back $= 1$, you hope that everything will converge and single out a nice submanifold” (McKean).
- The use of the term “slow manifold” for the case $\epsilon = 1$ seems to be an abuse of language. We can look for the invariant manifolds without slowness.
- We can study rescaled solutions instead of slow manifolds. (Very small velocities, very small gradients.)

Elusive slow manifold

- Invariance of a manifold is a local property: a vector field is tangent to a manifold
- Slowness of a manifold is not invariant with respect to diffeomorphisms: in a vicinity of a regular point ($J(x_0) \neq 0$) the existence and uniqueness theorems for $\dot{x} = J(x)$ mean that the vector field can be transformed to a constant $J(x) = J(x_0)$ in a vicinity of x_0 by a diffeomorphism.
- No slowness is possible for a constant field.
- Near fixed points ($x = 0$) linear systems $\dot{x} = Ax$ have slow manifolds – invariant subspace of A which correspond to the slower parts of spectrum.
- How can we continue these manifolds to the “nonlinear vicinity” of a fixed point?

Invariance


Invariance equation
dΨ/dt=J(Ψ)
J(Ψ)
T_Ψ Ω
Δ
Ψ
PJ(Ψ)
Ω – Ansatz
Manifold
Invariance equation
Δ=J-PJ=0

Analyticity instead of smallness (Lyapunov)

- The problem of the invariant manifold includes two difficulties: (i) it is difficult to find any global solution or even prove its existence and (ii) there often exists too many different local solutions.
- Lyapunov used the *analyticity* of the invariant manifold to prove its existence and uniqueness in some finite-dimensional problems (under “no resonance” conditions).
- Analyticity can be employed as a *selection criterion*.

Linear systems: analyticity selects eigenspaces

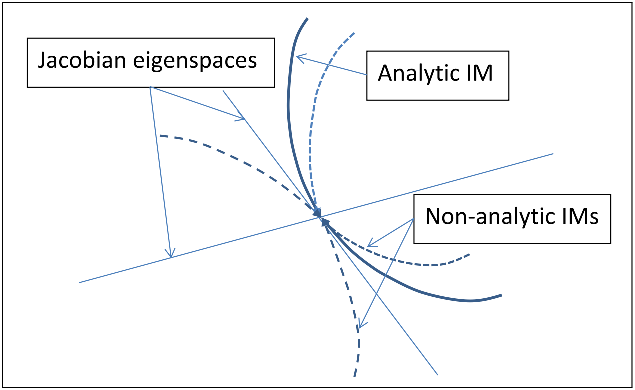
$$\frac{dx_1}{dt} = -\lambda_1 x_1$$
$$\frac{dx_2}{dt} = -\lambda_2 x_2$$

$x_i = A_i \exp(-\lambda_i t)$. If both $\lambda_i > 0$, λ_1/λ_2 is irrational (no resonances), and both $A_i \neq 0$ then the trajectory

$$\left(\frac{x_1}{A_1}\right)^{\lambda_2/\lambda_1} = \left(\frac{x_2}{A_2}\right)$$

is not analytic at $(0,0)$.
For linear systems without resonances
analyticity selects eigenspaces.

Lyapunov auxiliary theorem (1892)



The only analytical invariant manifold is tangent to some Jacobian eigenspace (with extension to some invariant spaces). For conditions – read Lyapunov.

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   - The Chapman–Enskog expansion

Rescaled weak solutions

1. A program of the derivation of (weak) solutions of the Navier–Stokes equations from the rescaled (weak) solutions of the Boltzmann equation was formulated in 1991 and finalized for incompressible fluids in 2004 with the answer:

- The incompressible Navier–Stokes (Navier–Stokes–Fourier) equations appear in a limit of appropriately scaled solutions of the Boltzmann equation.

(C. Bardos, F. Golse, D. Levermore, P.-L. Lions, N. Masmoudi, L. Saint-Raymond)
There remain some open questions for compressible case.

Invariant manifolds: power series

2. The invariant manifold approach to the kinetic part of the 6th Hilbert’s problem was invented by Enskog (1916)

- The Chapman–Enskog method aims to construct the invariant manifold for the Boltzmann equation in the form of a series in powers of a small parameter, the Knudsen number *Kn*.
- This invariant manifold is parameterized by the hydrodynamic fields (density, velocity, temperature). The zeroth-order term of this series is the local equilibrium.
- The zeroth term gives Euler equations, the first term gives the Navier–Stokes–Fourier hydrodynamics.
- The higher terms all are singular!

Invariant manifolds: direct iteration methods and exact solutions

- If we apply the Newton–Kantorovich method to the invariant manifold problem then the Chapman–Enskog singularities vanish (G&K, 1991-1994) but the convergence problem remains open.
- The algebraic and stable global invariant manifolds exist for some kinetic PDE (G&K, 1996-2002).

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The equation in abstract form

The invariance equation just expresses the fact that the vector field is tangent to the manifold.

- Let us consider an analytical vector field in a domain U of a space E with analytical right hand sides

$$\partial_t f = J(f).$$

- A space of macroscopic variables (moments) is defined with a surjective linear map to them $m : f \mapsto M$ (M are macroscopic variables).
- The self-consistency condition $m(\boldsymbol{f}_M) = M$.

The invariance equation

$$\boxed{J(\boldsymbol{f}_M) = (D_M \boldsymbol{f}_M) m(J(\boldsymbol{f}_M)).}$$

The differential D_M of $\boldsymbol{f}_M$ is calculated at $M = m(\boldsymbol{f}_M)$.

Micro- and macro- time derivatives

For an approximate invariant manifold $\boldsymbol{f}_M$ the approximate reduced model (projected equation) is

$$\partial_t M = m(J(\boldsymbol{f}_M)).$$

Invariance equation means that the time derivative of $\boldsymbol{f}$ on the manifold $\boldsymbol{f}_M$ can be calculated by a simple chain rule:

- Write that the time dependence of $\boldsymbol{f}$ can be expressed through the time dependence of M:

$$\partial_t^{\rm micro} \boldsymbol{f}_M = \partial_t^{\rm macro} \boldsymbol{f}_M,$$

- The microscopic time derivative is just a value of the vector field, $\partial_t^{\rm micro} \boldsymbol{f}_M = J(\boldsymbol{f}_M)$,
- The macroscopic time derivative is calculated by the chain rule, $\partial_t^{\rm macro} \boldsymbol{f}_M = (D_M \boldsymbol{f}_M) \partial_t M$ under the assumption that dynamics of M follows the projected equation.

Outline

The singularly perturbed system

A one-parametric system of equations is considered:

$$\partial_t f + A(f) = \frac{1}{\epsilon} Q(f).$$

The assumptions about the macroscopic variables $M = m(f)$:

- $m(Q(f)) \equiv 0$;
- for each $M \in m(U)$ the system of equations

$$Q(f) = 0, \quad m(f) = M$$

  has a unique solution $\boldsymbol{f}_M^{\mathrm{eq}}$ ("local equilibrium").

Fast subsystem

The fast system

$$\partial_t f = \frac{1}{\epsilon} Q(f)$$

should have the properties:

- $\boldsymbol{f}_M^{\mathrm{eq}}$ is asymptotically stable and globally attracting in $(\boldsymbol{f}_M^{\mathrm{eq}} + \ker m) \cap U$.
- The differential of the fast vector field $Q(f)$ at equilibrium $\boldsymbol{f}_M^{\mathrm{eq}}$, $\mathcal{Q}_M$ is invertible in $\ker m$, i.e. the equation $\mathcal{Q}_M \psi = \phi$ has a solution $\psi = (\mathcal{Q}_M)^{-1} \phi \in \ker m$ for every $\phi \in \ker m$.

The formal invariance equation

The invariance equation for the singularly perturbed system with the moment parametrization m is:

$$\boxed{\frac{1}{\epsilon}Q(\boldsymbol{f}_M) = A(\boldsymbol{f}_M) - (D_M\boldsymbol{f}_M)(m(A(\boldsymbol{f}_M))).}$$

We look for the invariant manifold in the form of the power series (Chapman–Enskog):

$$\boldsymbol{f}_M = \boldsymbol{f}_M^{\mathrm{eq}} + \sum_{i=1}^{\infty} \epsilon^i \boldsymbol{f}_M^{(i)}$$

With the self-consistency condition $m(\boldsymbol{f}_M) = M$ the first term of the Chapman–Enskog expansion is

$$\boxed{\boldsymbol{f}_M^{(1)} = \mathcal{Q}_M^{-1}(1 - (D_M\boldsymbol{f}_M^{\mathrm{eq}})m)(A(\boldsymbol{f}_M^{\mathrm{eq}})).}$$

Outline

4. Exact summation and capillarity of ideal gas
   - Chapman–Enskog series for the simplest model
   - Exact formulas for hydrodynamic stress and energy

The simplest model

$$\partial_t p = -\frac{5}{3}\partial_x u,$$
$$\partial_t u = -\partial_x p - \partial_x \sigma,$$
$$\partial_t \sigma = -\frac{4}{3}\partial_x u - \frac{1}{\epsilon}\sigma,$$

where x is the space coordinate (1D), $\boldsymbol{u}(x)$ is the velocity oriented along the x axis; σ is the dimensionless xx-component of the stress tensor.

- This is a simple linear system and can be integrated immediately in explicit form.
- Instead, we are interested in extracting the slow manifold by a direct method.

$$\boldsymbol{f} = \begin{pmatrix} p(x) \\ u(x) \\ \sigma(x) \end{pmatrix}, \; m = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \; M = \begin{pmatrix} p(x) \\ u(x) \end{pmatrix},$$

$$A(\boldsymbol{f}) = \begin{pmatrix} \frac{5}{3}\partial_x u \\ \partial_x p + \partial_x \sigma \\ \frac{4}{3}\partial_x u \end{pmatrix}, \; Q(\boldsymbol{f}) = \begin{pmatrix} 0 \\ 0 \\ -\sigma \end{pmatrix}, \; \ker m = \left\{ \begin{pmatrix} 0 \\ 0 \\ y \end{pmatrix} \right\},$$

$$\boldsymbol{f}_M^{\mathrm{eq}} = \begin{pmatrix} p(x) \\ u(x) \\ 0 \end{pmatrix}, \; D_M \boldsymbol{f}_M^{\mathrm{eq}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix}, \; \boldsymbol{f}_M^{(1)} = \begin{pmatrix} 0 \\ 0 \\ -\frac{4}{3}\partial_x u \end{pmatrix}.$$

$\mathcal{Q}_M^{-1} = \mathcal{Q}_M = -1$ on $\ker m$.

Invariance equation $\frac{1}{\epsilon} Q(\boldsymbol{f}_M) = A(\boldsymbol{f}_M) - (D_M \boldsymbol{f}_M)(m(A(\boldsymbol{f}_M)))$.

The invariance equation for the simplest model

$$-\frac{1}{\epsilon}\sigma_{(p,u)} = \frac{4}{3}\partial_x u - \frac{5}{3}(D_p\sigma_{(p,u)})(\partial_x u) - (D_u\sigma_{(p,u)})(\partial_x p + \partial_x \sigma_{(p,u)}).$$

Here, $M = (p, u)$ and the differentials are calculated by the elementary rule: if a function $\Phi = \Phi(p, \partial_x p, \partial_x^2 p, \dots)$ then

$$D_p\Phi = \frac{\partial\Phi}{\partial p} + \frac{\partial\Phi}{\partial(\partial_x p)}\partial_x + \frac{\partial\Phi}{\partial(\partial_x^2 p)}\partial_x^2 + \dots$$

The Chapman–Enskog expansion: $\sigma^{(0)}_{(p,u)} = 0$, $\sigma^{(1)}_{(p,u)} = -\frac{4}{3}\partial_x u$,

$$\sigma^{(i+1)}_{(p,u)} = \frac{5}{3}(D_p\sigma^{(i)}_{(p,u)})(\partial_x u) + (D_u\sigma^{(i)}_{(p,u)})(\partial_x p) + \sum_{j+l=i}(D_u\sigma^{(j)}_{(p,u)})(\partial_x\sigma^{(l)}_{(p,u)})$$

Truncated series

Projected equations

(Euler) $$\begin{aligned} \partial_t p &= -\tfrac{5}{3}\partial_x u, \\ \partial_t u &= -\partial_x p; \end{aligned}$$

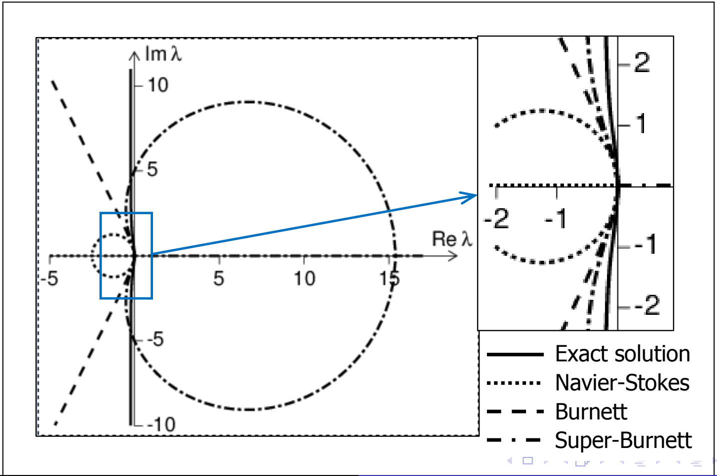
(Navier-Stokes) $$\begin{aligned} \partial_t p &= -\tfrac{5}{3}\partial_x u, \\ \partial_t u &= -\partial_x p + \epsilon\tfrac{4}{3}\partial_x^2 u. \end{aligned}$$

$$\begin{aligned} \partial_t p &= -\tfrac{5}{3}\partial_x u, \\ \partial_t u &= -\partial_x p + \epsilon\tfrac{4}{3}\partial_x^2 u + \epsilon^2\tfrac{4}{3}\partial_x^3 p \end{aligned}$$ (Burnett).

$$\begin{aligned} \partial_t p &= -\tfrac{5}{3}\partial_x u, \\ \partial_t u &= -\partial_x p + \epsilon\tfrac{4}{3}\partial_x^2 u + \epsilon^2\tfrac{4}{3}\partial_x^3 p + \epsilon^3\tfrac{4}{9}\partial_x^4 u \end{aligned}$$ (super Burnett).

Bobylev instability, and saturation of dissipation.1

Solution in the form $\exp(\lambda t + ikx)$



Bobylev instability, and saturation of dissipation. 2

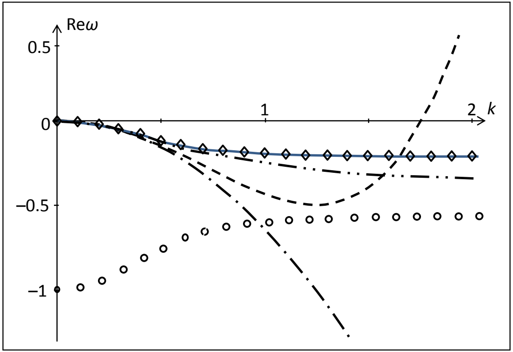


Figure: Solid: exact summation; diamonds: hydrodynamic modes of the simplest model with $\epsilon = 1$; circles: the non-hydrodynamic mode of this model; dash dot line: the Navier–Stokes approximation; dash: the super–Burnett approximation; dash double dot line: the first Newton's iteration.

Outline

4. Exact summation and capillarity of ideal gas
   - Chapman–Enskog series for the simplest model
   - Exact formulas for hydrodynamic stress and energy

The pseudodifferential form of stress tensor

Do not truncate the series!

The representation of σ on the hydrodynamic invariant manifold follows from the symmetry properties (u is a vector and p is a scalar):

$$\sigma(x) = A(-\partial_x^2)\partial_x u(x) + B(-\partial_x^2)\partial_x^2 p(x),$$

where $A(y)$, $B(y)$ are yet unknown analytical functions.
The invariance equation reduces to a system of two quadratic equations for functions $A(k^2)$ and $B(k^2)$:

$$-A - \frac{4}{3} - k^2\left(\frac{5}{3}B + A^2\right) = 0,$$

$$-B + A\left(1 - k^2 B\right) = 0.$$

It is analytically solvable! **We do not need series at all.**

The energy formula and capillarity of ideal gas

The standard energy formula is

$$\frac{1}{2}\partial_t\left(\frac{3}{5}\int_{-\infty}^{\infty} p^2\,\mathrm{d}x + \int_{-\infty}^{\infty} u^2\,\mathrm{d}x\right) = \int_{-\infty}^{\infty} \sigma\partial_x u\,\mathrm{d}x$$

On the invariant manifold

$$\boxed{\begin{aligned}\frac{1}{2}\partial_t\int_{-\infty}^{\infty}\left(\frac{3}{5}p^2 + u^2 - \frac{3}{5}(\partial_x p)(B(-\partial_x^2)\partial_x p)\right)\,\mathrm{d}x \\ = \int_{-\infty}^{\infty}(\partial_x u)(A(-\partial_x^2)\partial_x u)\,\mathrm{d}x\end{aligned}}$$

$$\begin{aligned}\partial_t(\text{MECHANICAL ENERGY}) + \partial_t(\text{CAPILLARITY ENERGY}) \\ = \text{VISCOUS DISSIPATION.}\end{aligned}$$

(Slemrod (2013) noticed that reduction of viscosity can be understood as appearance of capillarity.)

Matched asymptotics: from $k^2 = 0$ to $k^2 = \infty$

Take $\varsigma = 1/k^2$. For the analytic solutions near $\varsigma = 0$ the Taylor series is: $A = \sum_{l=1}^{\infty} \alpha_l \varsigma^l$, $B = \sum_{l=1}^{\infty} \beta_l \varsigma^l$, where $\alpha_1 = -\frac{4}{9}$, $\beta_1 = -\frac{4}{5}$, $\alpha_2 = \frac{80}{2187}$, $\beta_2 = \frac{4}{27}$,...
Already the first term gives for the frequency the proper limit:

$$\lambda_{\pm} = -\frac{2}{9} \pm i|k|\sqrt{3},$$

Matching this asymptotic with first terms at $k = 0$, we get

$$A \approx -\frac{4}{3+9k^2}, \quad B \approx -\frac{4}{3+5k^2}$$

and

$$\sigma_k = ikA(k^2)u_k - k^2B(k^2)p_k \approx -\frac{4ik}{3+9k^2}u_k + \frac{4k^2}{3+5k^2}p_k.$$

Reduced equations

For the stress tensor $\sigma(x) = A(-\partial_x^2)\partial_x u(x) + B(-\partial_x^2)\partial_x^2 p(x)$, the reduced equations have the form

$$\partial_t p = -\frac{5}{3}\partial_x u,$$
$$\partial_t u = -\partial_x p - \partial_x[A(-\partial_x^2)\partial_x u + B(-\partial x^2)\partial_x^2 p],$$

For the matched asymptotics

$$\partial_t p = -\frac{5}{3}\partial_x u,$$
$$(1-3\partial_x^2)\left(1-\frac{5}{3}\partial_x^2\right)\partial_t u$$
$$= -\partial_x p + \frac{4}{3}\partial_x\left[\left(1-\frac{5}{3}\partial_x^2\right)\partial_x u + (1-3\partial_x^2)\partial_x^2 p\right],$$

For the simple kinetic model:

- The Chapman–Enskog series amounts to an algebraic invariant manifold, and the “smallness" of the Knudsen number ϵ *is not necessary*.
- The exact dispersion relation on the algebraic invariant manifold *is stable for all wave lengths*.
- The exact hydrodynamics are *essentially nonlocal* in space.
- The Newton iterations for the invariance equations provide *much better results* than the Chapman–Enskog expansion.
- In the exact energy equation *the capillarity term* appears.

Outline

The Grad 13 moment systems provides the simplest coupling of the hydrodynamic variables ρ_k, u_k, and T_k to stress tensor σ_k and heat flux q_k. In 1D

$$
\begin{aligned}
\partial_t \rho_k &= -iku_k, \\
\partial_t u_k &= -ik\rho_k - ikT_k - ik\sigma_k, \\
\partial_t T_k &= -\frac{2}{3}iku_k - \frac{2}{3}ikq_k, \\
\partial_t \sigma_k &= -\frac{4}{3}iku_k - \frac{8}{15}ikq_k - \sigma_k, \\
\partial_t q_k &= -\frac{5}{2}ikT_k - ik\sigma_k - \frac{2}{3}q_k.
\end{aligned}
$$

We use the symmetry properties and find the representation of σ, q:

$$\sigma_k = ikA(k^2)u_k - k^2B(k^2)\rho_k - k^2C(k^2)T_k,$$
$$q_k = ikX(k^2)\rho_k + ikY(k^2)T_k - k^2Z(k^2)u_k,$$

where the functions $A, \dots, Z$ are the unknowns in the invariance equation.
After elementary transformations we find the invariance equation.

The invariance equation for this case is a system of six coupled quadratic equations with quadratic in k^2 coefficients:

$$\begin{aligned}
-\frac{4}{3} - A - k^2\left(A^2 + B - \frac{8Z}{15} + \frac{2C}{3}\right) + \frac{2}{3}k^4 CZ &= 0,\\
\frac{8}{15}X + B - A + k^2 AB + \frac{2}{3}k^2 CX &= 0,\\
\frac{8}{15}Y + C - A + k^2 AC + \frac{2}{3}k^2 CY &= 0,\\
A + \frac{2}{3}Z + k^2 ZA - X - \frac{2}{3}Y + \frac{2}{3}k^2 YZ &= 0,\\
k^2 B - \frac{2}{3}X - k^2 Z + k^4 ZB - \frac{2}{3}YX &= 0,\\
-\frac{5}{2} - \frac{2}{3}Y + k^2(C - Z) + k^4 ZC - \frac{2}{3}k^2 Y^2 &= 0.
\end{aligned}$$

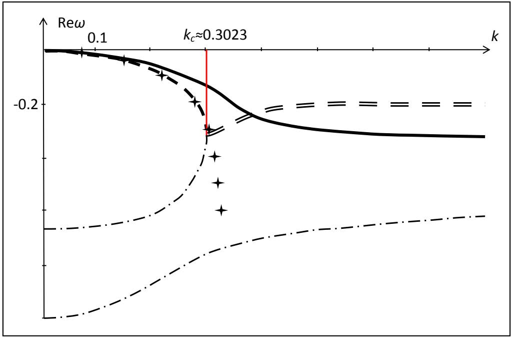


Figure: The bold solid line shows the acoustic mode (two complex conjugated roots). The bold dashed line is the diffusion mode (a real root). At $k = k_c$ it meets a real root of non-hydrodynamic mode (dash-dot line) and for $k > k_c$ they turn into a couple of complex conjugated roots (double-dashed line). The stars – the third Newton iteration (diffusion mode). Dash-and-dot – non-hydrodynamic modes.

Outline

5. Examples and problems
   - Destruction of hydrodynamic invariant manifold for short waves
   - Approximate invariant manifold for the Boltzmann equation
   - The projection problem and the entropy equation

The equation and macroscopic variables

The Boltzmann equation in a co-moving reference frame,

$$D_t f = -(\boldsymbol{v} - \boldsymbol{u}) \cdot \nabla_x f + Q(f),$$

where $D_t = \partial_t + \boldsymbol{u} \cdot \nabla_x$. The macroscopic variables are:

$$M = \left\{ n; n\boldsymbol{u}; \frac{3nk_{\mathrm{B}}T}{\mu} + nu^2 \right\} = m[f] = \int \{1; \boldsymbol{v}; v^2\} f \, \mathrm{d}\boldsymbol{v},$$

These fields do not change in collisions, hence, the projection of the Boltzmann equation on the hydrodynamic variables is

$$D_t M = -m[(\boldsymbol{v} - \boldsymbol{u}) \cdot \nabla_x f].$$

The problem

- We are looking for invariant manifold $\boldsymbol{f}_M$ in the space of distribution functions parameterized by the hydrodynamic fields.
- Such a manifold is represented by a lifting map $M \mapsto f_M$.
- It maps three functions of the space variables, $M = \{n(\boldsymbol{x}), \boldsymbol{u}(\boldsymbol{x}), T(\boldsymbol{x})\}$, into a function of six variables $\boldsymbol{f}_M(\boldsymbol{x}, \boldsymbol{v})$.
- The consistency condition should hold: $m[f_M] = M$.
- The zero approximation for $\boldsymbol{f}_M$ give the local Maxwellians.

The invariance equation

For the Boltzmann equation,

$$D_t^{\mathrm{micro}} f_M = -(\boldsymbol{v} - \boldsymbol{u}) \cdot \nabla_x f_M + Q(f_M),$$

$$D_t^{\mathrm{macro}} f_M = -(D_M f_M) m[(\boldsymbol{v} - \boldsymbol{u}) \cdot \nabla_x f_M].$$

The invariance equation

$$D_t^{\mathrm{micro}} f_M = D_t^{\mathrm{macro}} f_M$$

$$\boxed{-(D_M \boldsymbol{f}_M) m[(\boldsymbol{v} - \boldsymbol{u}) \cdot \nabla_x \boldsymbol{f}_M] = -(\boldsymbol{v} - \boldsymbol{u}) \cdot \nabla_x \boldsymbol{f}_M + Q(\boldsymbol{f}_M)}.$$

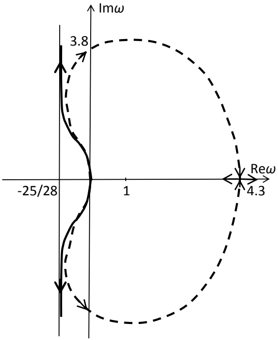
- We solve it by the Newton–Kantorovich method;
- We use the microlocal analysis to solve the differential equations at each iteration.

$$
\begin{aligned}
\sigma(x) = & -\frac{1}{6\pi} n(x) \int_{-\infty}^{+\infty} \mathrm{d}y \int_{-\infty}^{+\infty} \mathrm{d}k \exp(ik(x-y)) \frac{2}{3} \partial_y u(y) \\
& \times \left[\left(n(x)\lambda_3 + \frac{11}{9} \partial_x u(x) \right) \left(n(x)\lambda_4 + \frac{27}{4} \partial_x u(x) \right) + \frac{k^2 v_T^2(x)}{9} \right]^{-1} \\
& \times \left[\left(n(x)\lambda_3 + \frac{11}{9} \partial_x u(x) \right) \left(n(x)\lambda_4 + \frac{27}{4} \partial_x u(x) \right) \right. \\
& + \frac{4}{9} \left(n(y)\lambda_4 + \frac{27}{4} \partial_y u(y) \right) v_T^{-2}(x) (u(x) - u(y))^2 \partial_x u(x) \\
& \left. - \frac{2}{3} ik (u(x) - u(y)) \partial_x u(x) \right] \left(n(y)\lambda_3 + \frac{11}{9} \partial_y u(y) \right)^{-1} \\
& + O\left(\partial_x \ln T(x), \partial_x \ln n(x) \right).
\end{aligned}
$$

Comment about the result of the first iteration for the stress tensor

- It is nonlinear and nonlocal.
- All the information about the collision model is collected in the numbers $\lambda_{3,4} > 0$. They are represented by quadratures.
- The ‘residual’ terms describe the part of the stress tensor governed by the temperature and density gradients.

For Maxwell's molecules near equilibrium



Solid line with saturation is Newton's iteration, dashed line is Burnett's approximation.

$$\sigma = -\frac{2}{3} n_0 T_0 \left(1 - \frac{2}{5}\partial_x^2\right)^{-1} \left(2\partial_x u - 3\partial_x^2 T\right);$$

$$q = -\frac{5}{4} n_0 T_0^{3/2} \left(1 - \frac{2}{5}\partial_x^2\right)^{-1} \left(3\partial_x T - \frac{8}{5}\partial_x^2 u\right).$$

Outline

5 Examples and problems
- Destruction of hydrodynamic invariant manifold for short waves
- Approximate invariant manifold for the Boltzmann equation
- The projection problem and the entropy equation

The projection problem: The general formulation

- The *exact* invariant manifolds inherit many properties of the original systems: conservation laws, dissipation inequalities (entropy growth) and hyperbolicity.
- In real-world applications, we usually should work with the *approximate* invariant manifolds.
- If $\boldsymbol{f}_M$ is not an exact invariant manifold then a special *projection problem* arises:

Define the projection of the vector field on the manifold $\boldsymbol{f}_M$ that preserves the conservation laws and the positivity of entropy production.

The projection problem: An example

- The first and the most successful ansatz for the shock layer is the bimodal Tamm–Mott-Smith (TMS) approximation:

$$f(\boldsymbol{v},\boldsymbol{x}) = f_{\mathrm{TMS}}(\boldsymbol{v},z) = a_-(z)f_-(\boldsymbol{v}) + a_+(z)f_+(\boldsymbol{v}),$$

  where $f_\pm(\boldsymbol{v})$ are the input and output Maxwellians.
- Most of the projectors used for TMS violate the second law: entropy production is sometimes negative.
- Lampis (1977) used the entropy density s as a new variable and solved this problem.

The thermodynamic projector: The formalized problem

Surprisingly, the proper projector is in some sense unique (G&K 1991, 2003).

- Let us consider all smooth vector fields with non-negative entropy production.
- The projector which preserves the nonnegativity of the entropy production for *all* such fields turns out to be unique. This is the so-called *thermodynamic projector*, P_T
- The projector P is defined for a given state f, closed subspace $T_f = \mathrm{im} P_T$, the differential $(DS)_f$ and the second differential $(D^2S)_f$ of the entropy S at f.

The thermodynamic projector: The answer

$$P_T(J) = P^{\perp}(J) + \frac{g^{\parallel}}{\langle g^{\parallel} | g^{\parallel} \rangle_f} \langle g^{\perp} | J \rangle_f,$$

where

- $\langle \bullet | \bullet \rangle_f$ is the entropic inner product at f: $\langle \phi | \psi \rangle_f = -(\phi, (D^2 S)_f \psi)$,
- $P_T^{\perp}$ is the orthogonal projector onto T_f with respect to the entropic scalar product,
- g is the Riesz representation of the linear functional $D_x S$ with respect to entropic scalar product: $\langle g, \varphi \rangle_f = (DS)_f(\varphi)$ for all φ, $g = g^{\parallel} + g^{\perp}$, $g^{\parallel} = P^{\perp} g$, and $g^{\perp} = (1 - P^{\perp}) g$.

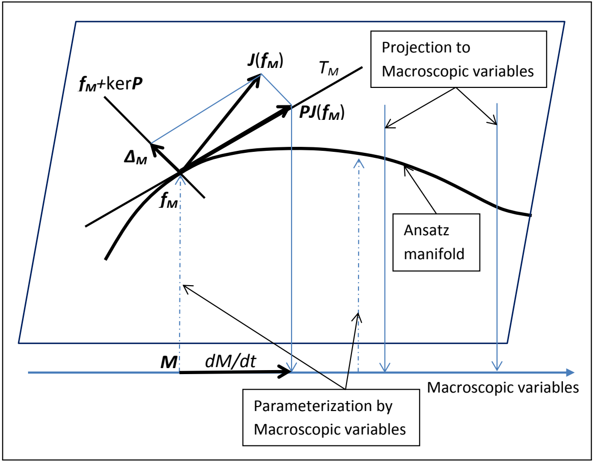


Figure: Geometry of the thermodynamic projector onto the *ansatz* manifold

The thermodynamic projector in quasi-equilibria

- For the quasi-equilibrium (MaxEnt), $\boldsymbol{f}_M$ is the entropy maximizer under given value of M.
- For the quasi-equilibrium (MaxEnt) ansatz the standard moment projection

$$\partial_t M = m(J(\boldsymbol{f}_M)).$$

  gives the same equations as the thermodynamic projector does.
- For the local equilibria the thermodynamic projector adds nothing new.

In general situation, the projected equations are not so simple as we have expected!

Main message

- It is useful to solve the invariance equation.
- Analyticity + zero-order term select the proper invariant manifold without use of a small parameter.
- Analytical invariant manifolds for kinetic PDE may exist, and the exact solutions demonstrate this on the simple equations.

Is this fragment of 6th Hilbert problem solved?

We can choose what we like from three answers.

- In some sense, yes, it is solved positively, for the weak rescaled solutions of the Boltzmann equation the incompressible classical hydrodynamic limit is proven.
- No, it is open, for the compressible limit there remain some difficulties.
- Yes, it is solved negatively: for the non-equilibrium systems hydrodynamic equations differ from the classical Navier–Stokes–Fourier equations.

If we have the appetite to new equations then we prefer the third answer.

Scaling kills the saturation of dissipation

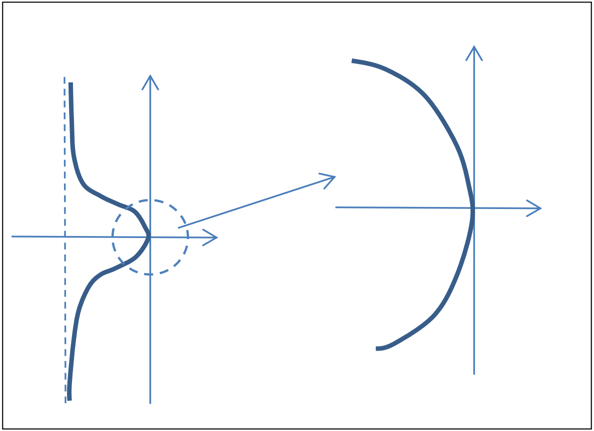


Figure: Everything scales to a parabola (or even to a straight line).

Three reviews and one note

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Thank you