

Exact and approximate hydrodynamic manifolds for kinetic equations

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Outline

- 1 Hilbert's 6th problem: From Boltzmann to hydrodynamics
 - Reduction problem
 - Two programs of the way “to the laws of motion of continua”
- 2 Invariance equation and Chapman–Enskog series
 - Invariance equation
 - The Chapman–Enskog expansion and exact solutions
- 3 Examples and problems
 - Destruction of hydrodynamic invariant manifold for short waves
 - Approximate invariant manifold for the Boltzmann equation
- 4 The projection problem

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From Boltzmann equation to fluid dynamics: Hilbert's 6th problem. Main technical questions

D. Hilbert: *“Boltzmann's work on the principles of mechanics suggests the problem of developing mathematically the limiting processes, there merely indicated, which lead from the atomistic view to the laws of motion of continua.”*

- 1 Is there hydrodynamics (hidden) in the kinetic equation?
- 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 $f(t, \mathbf{x}; \mathbf{v})$

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

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

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

McKean diagram (1965) (IM=Invariant Manifold)

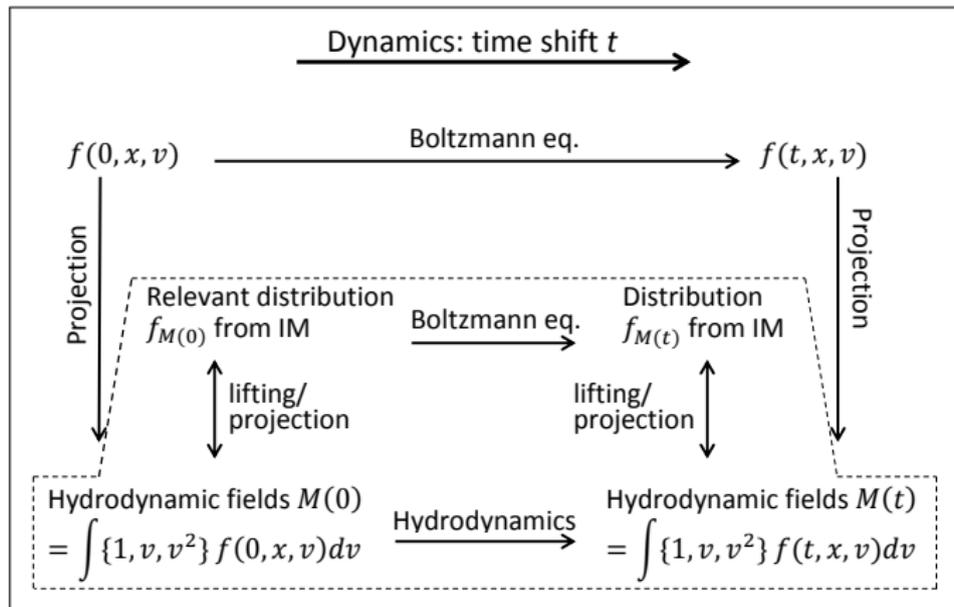
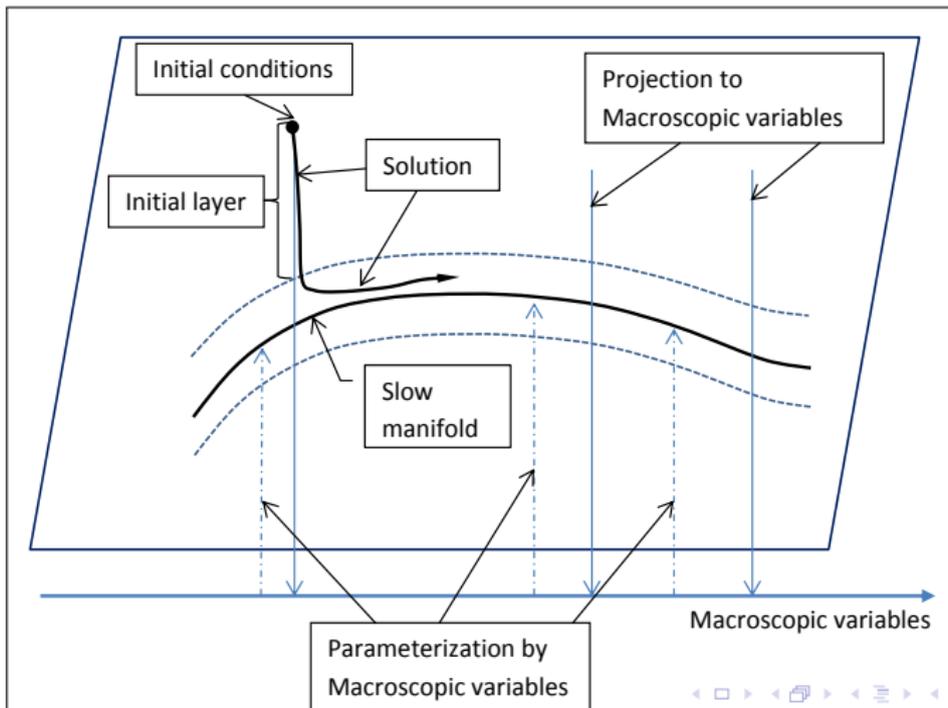


Figure: The diagram in the dashed polygon is commutative.

Singular perturbations and slow manifold diagram



The doubt about small parameter (McKean, Slemrod)

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

- 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).

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 vector field can be transformed to a constant $J(x) = J(x_0)$ in a by a diffeomorphism.

BUT

- 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?

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*.

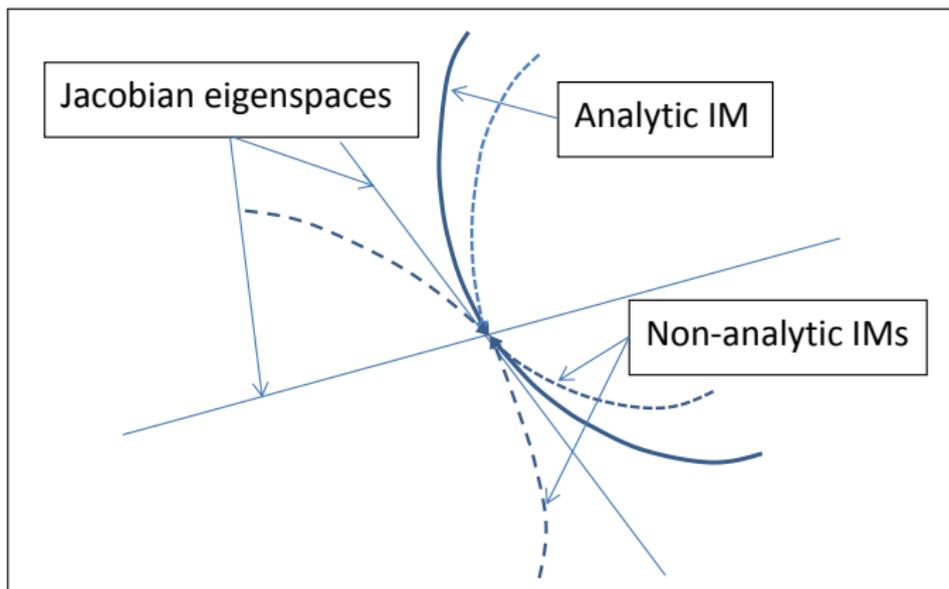


Figure: Lyapunov auxiliary theorem (1892).

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Rescaled weak solutions

(C. Bardos, F. Golse, D. Levermore, P.-L. Lions, N. Masmoudi, L. Saint-Raymond)

- The incompressible Navier–Stokes equations appear in a limit of appropriately scaled solutions of the Boltzmann equation.
- These solutions are infinitely slow and with infinitely small gradients (rescaled then back to normal velocities and gradients).

Invariant manifolds: power series

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 \Leftrightarrow vector field is tangent to the manifold.

- J is an analytical vector field in a domain U of a space E

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

- Macroscopic variables M (moments) are defined with a surjective linear map $m : f \mapsto M$ (M are macroscopic variables).
- We are looking for a manifold \mathbf{f}_M .
- The self-consistency condition $m(\mathbf{f}_M) = M$.

The invariance equation

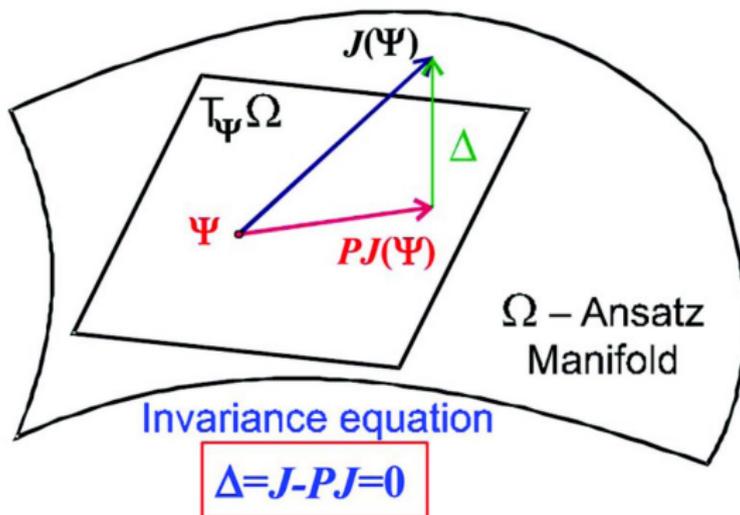
$$J(\mathbf{f}_M) = (D_M \mathbf{f}_M) m(J(\mathbf{f}_M)).$$

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

Invariance

Invariance equation

$$d\Psi/dt = J(\Psi)$$



Micro- and macro- time derivatives

The approximate projected equation is

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

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

- The time derivative of \mathbf{f} can be expressed through the projected time derivative of M :

$$\partial_t^{\text{micro}} \mathbf{f}_M = \partial_t^{\text{macro}} \mathbf{f}_M,$$

- The microscopic time derivative is just a value of the vector field, $\partial_t^{\text{micro}} \mathbf{f}_M = J(\mathbf{f}_M)$,
- The macroscopic time derivative is calculated by the chain rule, $\partial_t^{\text{macro}} \mathbf{f}_M = (D_M \mathbf{f}_M) \partial_t M = (D_M \mathbf{f}_M) m(J(\mathbf{f}_M))$

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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 f_M^{eq} (“local equilibrium”).

Fast subsystem

The fast system

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

should have the properties:

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

The C-E solution of the formal invariance equation

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

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

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

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

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

$$\mathbf{f}_M^{(1)} = Q_M^{-1}(1 - (D_M \mathbf{f}_M^{\text{eq}})m)(A(\mathbf{f}_M^{\text{eq}})).$$

The simplest model

$$\begin{aligned}\partial_t \rho &= -\frac{5}{3} \partial_x u, \\ \partial_t u &= -\partial_x \rho - \partial_x \sigma, \\ \partial_t \sigma &= -\frac{4}{3} \partial_x u - \frac{1}{\epsilon} \sigma,\end{aligned}$$

where x is the space coordinate (1D), $\mathbf{u}(x)$ 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.

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

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

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

$$Q_M^{-1} = Q_M = -1 \text{ on } \ker m.$$

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

The invariance equation for the simplest model

The invariance equation

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

The Chapman–Enskog expansion:

- $\sigma_{(p,u)}^{(0)} = 0,$
- $\sigma_{(p,u)}^{(1)} = -\frac{4}{3}\partial_x u,$
- $\sigma_{(p,u)}^{(i+1)} = \frac{5}{3}(D_p\sigma_{(p,u)}^{(i)})(\partial_x u) + (D_u\sigma_{(p,u)}^{(i)})(\partial_x p) + \sum_{j+l=i} (D_u\sigma_{(p,u)}^{(j)})(\partial_x\sigma_{(p,u)}^{(l)})$

Truncated series

Projected equations

$$\begin{aligned} \text{(Euler)} \quad \partial_t \mathbf{p} &= -\frac{5}{3} \partial_x u, & \text{(Navier-Stokes)} \quad \partial_t \mathbf{p} &= -\frac{5}{3} \partial_x u, \\ \partial_t u &= -\partial_x \mathbf{p}; & \partial_t u &= -\partial_x \mathbf{p} + \epsilon \frac{4}{3} \partial_x^2 u. \end{aligned}$$

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

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

The pseudodifferential form of σ

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 $B(k^2)$:

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

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

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

Attenuation rates

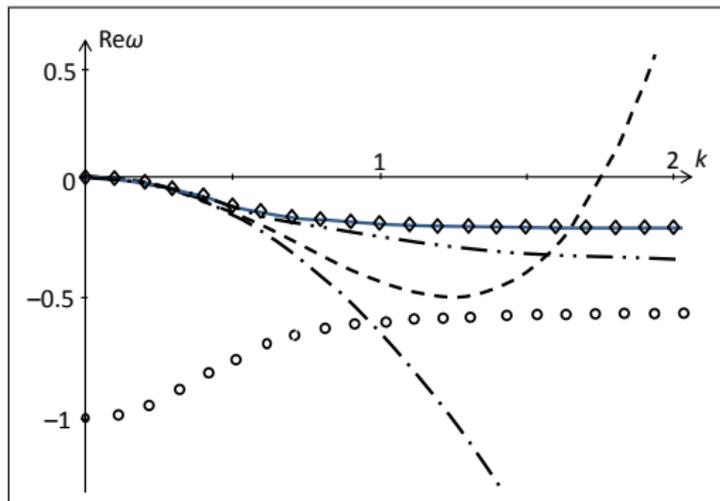


Figure: Solid: exact summation; diamonds: hydrodynamic modes of the simplest model with $\epsilon = 1$; circles: the non-hydrodynamic mode of this model; dash dot line: the Navier–Stokes approximation; dash: the super–Burnett approximation; dash double dot line: the first Newton's

The standard energy formula is

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

On the invariant manifold

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

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

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

For the simple kinetic model:

- The Chapman–Enskog series amounts to an algebraic invariant manifold.
- 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.
- In the exact energy equation *the capillarity term* appears.

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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

$$\partial_t \rho_k = -iku_k,$$

$$\partial_t u_k = -ik\rho_k - ikT_k - ik\sigma_k,$$

$$\partial_t T_k = -\frac{2}{3}iku_k - \frac{2}{3}ikq_k,$$

$$\partial_t \sigma_k = -\frac{4}{3}iku_k - \frac{8}{15}ikq_k - \sigma_k,$$

$$\partial_t q_k = -\frac{5}{2}ikT_k - ik\sigma_k - \frac{2}{3}q_k.$$

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

$$\begin{aligned}\sigma_k &= ikA(k^2)u_k - k^2B(k^2)\rho_k - k^2C(k^2)T_k, \\ q_k &= ikX(k^2)\rho_k + ikY(k^2)T_k - k^2Z(k^2)u_k,\end{aligned}$$

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:

$$-\frac{4}{3} - A - k^2(A^2 + B - \frac{8Z}{15} + \frac{2C}{3}) + \frac{2}{3}k^4CZ = 0,$$

$$\frac{8}{15}X + B - A + k^2AB + \frac{2}{3}k^2CX = 0,$$

$$\frac{8}{15}Y + C - A + k^2AC + \frac{2}{3}k^2CY = 0,$$

$$A + \frac{2}{3}Z + k^2ZA - X - \frac{2}{3}Y + \frac{2}{3}k^2YZ = 0,$$

$$k^2B - \frac{2}{3}X - k^2Z + k^4ZB - \frac{2}{3}YX = 0,$$

$$-\frac{5}{2} - \frac{2}{3}Y + k^2(C - Z) + k^4ZC - \frac{2}{3}k^2Y^2 = 0.$$

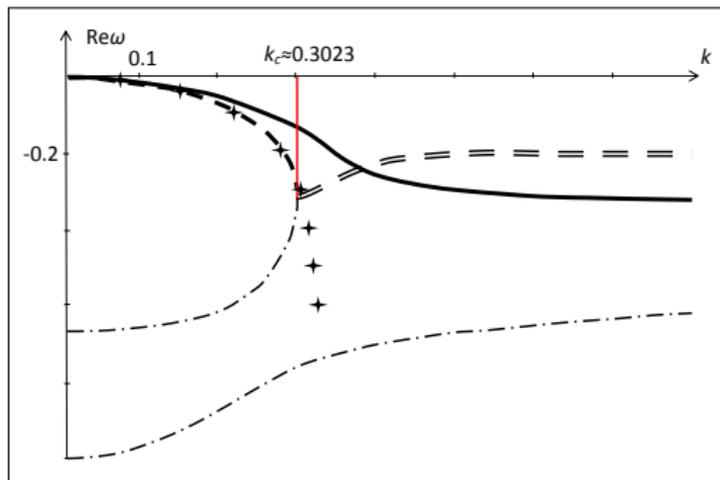


Figure: The bold solid line shows the acoustic mode (two complex conjugated roots). The bold dashed line is the diffusion mode (a real root). At $k = k_c$ it meets a real root of non-hydrodynamic mode (dash-dot line) and for $k > k_c$ they turn into a couple of complex conjugated roots (double-dashed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

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The equation and macroscopic variables

The Boltzmann equation in a co-moving reference frame,

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

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

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

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

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

The invariance equation

For the Boltzmann equation,

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

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

The invariance equation

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

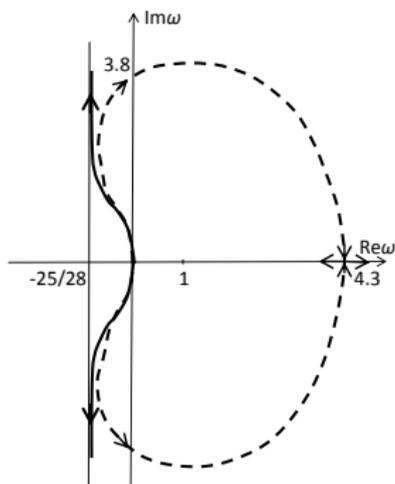
$$\boxed{-(D_M \mathbf{f}_M) m[(\mathbf{v} - \mathbf{u}) \cdot \nabla_x \mathbf{f}_M] = -(\mathbf{v} - \mathbf{u}) \cdot \nabla_x \mathbf{f}_M + Q(\mathbf{f}_M)}.$$

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

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

For Maxwell's molecules near equilibrium

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



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

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

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 \mathbf{f}_M is not an exact invariant manifold then a special *projection problem* arises:

Define the projection of the vector field on the manifold \mathbf{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:

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

where $f_{\pm}(\mathbf{v})$ 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 $T_f = \text{im}P_T$, 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 $g^\perp = (1 - P^\perp)g$.

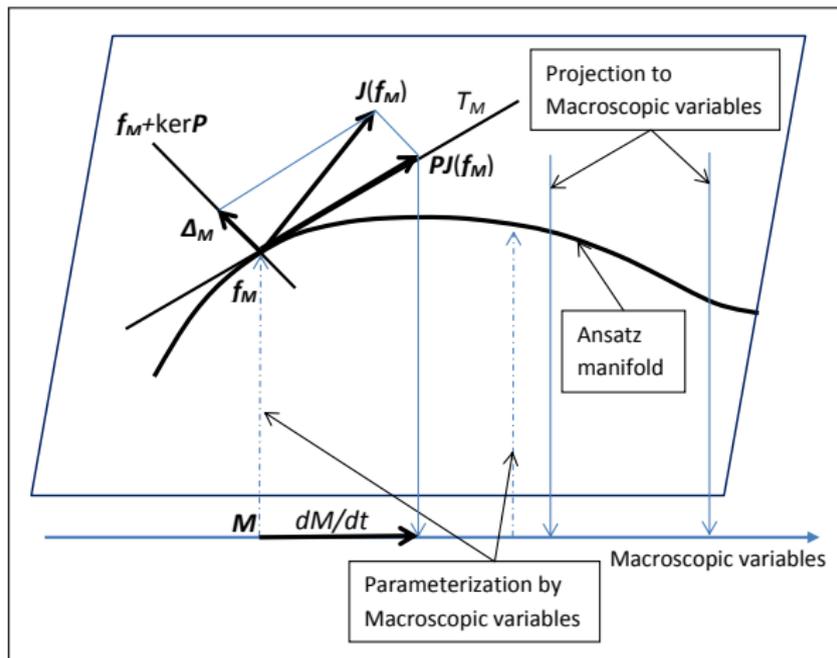


Figure: Geometry of the thermodynamic projector onto the *ansatz* manifold

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.

Two reviews and one note

- 1 A.N. Gorban, I. Karlin, **Hilbert's 6th Problem: exact and approximate hydrodynamic manifolds for kinetic equations**, Bulletin of the American Mathematical Society **51** (2), 2014, 186–246.
- 2 M. Slemrod, **From Boltzmann to Euler: Hilbert's 6th problem revisited**, Computers and Mathematics with Applications **65** (2013), no. 10, 1497–1501. And **Slemrod talk in Oxford, October, 2012**.
- 3 A.N. Gorban, I.V. Karlin **Beyond Navier–Stokes equations: capillarity of ideal gas**, Contemporary Physics **58** (1) (2017), 70–90,
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Hilbert's 6th problem: From Boltzmann to hydrodynamics
Invariance equation and Chapman–Enskog series
Examples and problems
The projection problem
Summary

Thank you



- “Model Reduction and Coarse-Graining Approaches for Multiscale Phenomena” University of Leicester, UK, August 24-26, 2005.
- “Principal manifolds for data cartography and dimension reduction” August 24-26, 2006, University of Leicester, UK.
- “ Mathematics of Model Reduction”, University of Leicester, UK August 28-30, 2007.
- “Coping with Complexity: Model Reduction and Data Analysis”, Ambleside, Lake District, UK, August 31 - September 4, 2009.
- “Model reduction across disciplines”, University of Leicester, UK, 19-22 of August 2014.
- “Hilbert’s Sixth Problem”, University of Leicester, UK, May 02-04, 2016.