

# Fluid Dynamics from Kinetic Equations

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*Fields Institute, 24–26 March 2004*

## OUTLINE

Lecture 1: Boltzmann to Euler (FG)

Lecture 2: More General Kinetic Settings (DL)

Lecture 3: Hilbert and Chapman-Enskog Expansions (FG)

Lecture 4: Linear and Weakly Nonlinear Fluid Dynamical Limits (DL)

Lecture 5: Global Solutions and Global Limits (DL)

Lecture 6: Incompressible Navier-Stokes Limit for Boltzmann (FG)

## **LECTURE 2:**

### **MORE GENERAL KINETIC SETTINGS**

- I. INTRODUCTION**
- II. PROPERTIES OF COLLISION OPERATORS**
- III. CONSEQUENCES OF THE PROPERTIES**
- IV. GENERAL COMPRESSIBLE EULER SYSTEMS**
- V. EXAMPLES**

## I. INTRODUCTION

We now consider a general class of kinetic theories that includes the classical Boltzmann equation. The goal is to show how concepts introduced in the first lecture apply in other settings.

We consider a gas of identical molecules where the state of each molecule is given by its position  $x \in \Omega \subset \mathbb{R}^D$  (where  $D = 3$  is of greatest interest) and its local state  $s$  in a state space  $S$  endowed with a measure  $d\sigma(s)$ .

There is a function  $v$  that to each local state  $s \in S$  assigns a velocity  $v(s) \in \mathbb{R}^D$ . This allows the same velocity to be assigned to different local states, thus enabling the introduction of internal degrees of freedom or other such devices that can extend the range of modeled phenomena.

## More General Kinetic Equations

The kinetic density  $F = F(s, x, t)$  represents the mass density over the single-molecule phase space  $S \times \Omega$  at time  $t$ . If  $A$  is any measurable subset of  $S \times \Omega$  then

$$\iint_A F(s, x, t) d\sigma(s) dx$$

gives the mass of fluid molecules in  $A$  at time  $t$ .

The evolution of  $F$  is assumed to be governed by

$$\partial_t F + v \cdot \nabla_x F = \mathcal{C}(F).$$

The so-called collision operator  $\mathcal{C}$  acts only on  $s$  and is generally nonlinear. It is assumed to be defined over a domain  $\text{Dom}(\mathcal{C}) \subset L^1(d\sigma)$  that is contained within the cone of non-negative functions.

## II. PROPERTIES OF COLLISION OPERATORS

The form of the associated fluid dynamical equations depends on structural properties of  $\mathcal{C}$  relating to concepts of equilibria, conservation, dissipation, and entropy. These properties, which are shared by a wide variety of collision operators, are given below and are subsequently applied to deriving the analog of the classical compressible Euler system.

We will denote the integral of any scalar-, vector-, or matrix-valued function  $\phi = \phi(s)$  over the variable  $s$  by  $\langle \phi \rangle$ :

$$\langle \phi \rangle = \int_S \phi(s) d\sigma(s) .$$

## Conservation Properties - 1

A function  $e = e(s)$  is said to be a locally conserved quantity for  $\mathcal{C}$  whenever  $ef \in L^1(d\sigma)$ ,  $e\mathcal{C}(f) \in L^1(d\sigma)$ , and

$$\langle e\mathcal{C}(f) \rangle = 0 \quad \text{for every } f \in \text{Dom}(\mathcal{C}).$$

These form a linear subspace  $\mathbb{E}$ . We *assume* that  $\mathbb{E}$  is nontrivial.

Often  $\mathbb{E}$  is spanned by quantities associated with classical conservation laws. For the Boltzmann equation

$$\mathbb{E} = \text{span}\{1, v_1, v_2, \dots, v_D, |v|^2\}.$$

## Conservation Properties - 2

More generally, let  $N$  be the dimension of  $\mathbb{E}$ , and let  $\{e_i : 1 \leq i \leq N\}$  be a basis for  $\mathbb{E} \subset \mathbb{R}^S$ . Then

$$\mathbb{E} = \text{span}\{e_i : 1 \leq i \leq N\}.$$

Let  $\mathbf{e}$  denote the column vector whose components are these basis functions.

These locally conserved quantities lead to the local conservation laws

$$\partial_t \langle \mathbf{e} F \rangle + \nabla_x \cdot \langle \mathbf{v} \mathbf{e} F \rangle = 0.$$

They are satisfied (formally) by every solution  $F$  of the kinetic equation. The components of  $\langle \mathbf{e} F \rangle$  and  $\langle \mathbf{v} \mathbf{e} F \rangle$  are the densities and fluxes corresponding to the components of  $\mathbf{e}$ .

## Entropy Dissipation Properties - 1

A function  $\eta = \eta(f)$  is said to be an entropy for  $\mathcal{C}$  whenever: it is strictly convex with  $\eta_{ff}(f) > 0$ ; it satisfies  $\eta(f) \in L^1(d\sigma)$ ,  $\eta_f(f) \mathcal{C}(f) \in L^1(d\sigma)$ , and

$$\langle \eta_f(f) \mathcal{C}(f) \rangle \leq 0, \quad \text{for every } f \in \text{Dom}(\mathcal{C});$$

and for every  $f \in \text{Dom}(\mathcal{C})$  the following are equivalent:

- (i)  $\langle \eta_f(f) \mathcal{C}(f) \rangle = 0,$
- (ii)  $\mathcal{C}(f) = 0,$
- (iii)  $\eta_f(f) \in \mathbb{E}.$

This abstracts some aspects of Boltzmann's celebrated  $H$ -theorem.

## Entropy Dissipation Properties - 2

We *assume* that  $\mathcal{C}$  has a distinguished entropy  $\eta$ . For the Boltzmann equation and many other classical kinetic theories this entropy is  $\eta(f) = f \log(f) - f$ .

This entropy leads to the local entropy dissipation law

$$\partial_t \langle \eta(F) \rangle + \nabla_x \cdot \langle v \eta(F) \rangle = \langle \eta_f(F) \mathcal{C}(F) \rangle \leq 0.$$

It is satisfied (formally) by every solution  $F$  of the kinetic equation. Here  $\langle \eta(F) \rangle$  and  $\langle v \eta(F) \rangle$  are the entropy density and entropy flux, while  $\langle \eta_f(F) \mathcal{C}(F) \rangle$  is the entropy dissipation rate.

## Existence of Equilibria Property

The  $H$ -theorem properties do not guarantee that for every  $f$  there exists an equilibrium that shares the same values of the conserved densities with  $f$ . Let  $\mathbf{R}$  denote those points in  $\mathbb{R}^N$  that are realizable as the conserved densities of some  $f$ :

$$\mathbf{R} \equiv \left\{ \boldsymbol{\rho} \in \mathbb{R}^N : \boldsymbol{\rho} = \langle \mathbf{e} f \rangle \text{ for some } f \in \text{Dom}(\mathcal{C}) \right\}.$$

We *assume* that for every  $\boldsymbol{\rho} \in \mathbf{R}$  there exists a unique  $\mathcal{E}(\boldsymbol{\rho}) \in \text{Dom}(\mathcal{C})$  that satisfies

$$\langle \mathbf{e} \mathcal{E}(\boldsymbol{\rho}) \rangle = \boldsymbol{\rho}, \quad \mathcal{C}(\mathcal{E}(\boldsymbol{\rho})) = 0.$$

In other words, for every  $f \in \text{Dom}(\mathcal{C})$  there is a local equilibrium  $\mathcal{E}(\boldsymbol{\rho})$  that is uniquely determined by the densities  $\boldsymbol{\rho} = \langle \mathbf{e} f \rangle$ .

### III. CONSEQUENCES OF THE PROPERTIES

We will adopt the following notational conventions. Products are matrix multiplication with the understanding that vectors in  $\mathbb{R}^N$  are column vectors, while those from  $\mathbb{R}^{N*}$  are row vectors. Gradients of scalars with respect to column vectors are row vectors, and vice versa.

The first consequence of the properties assumed for  $\mathcal{C}$  is that one can find a formula for the family of equilibria  $\mathcal{E}(\rho)$ .

Because the components of  $\mathbf{e}$  are a basis for  $\mathbb{E}$ , one has that  $e \in \mathbb{E}$  if and only if  $e = \beta \mathbf{e}$  for a unique  $\beta \in \mathbb{R}^{N*}$ . Hence, characterization (iii) becomes

$$\eta_f(f) = \beta \mathbf{e}, \quad \text{for some } \beta \in \mathbb{R}^{N*}.$$

This can be solved for  $f$  in terms of the Legendre transform of  $\eta$ , denoted by  $\eta^* = \eta^*(z)$ .

## The Legendre Transform of $\eta$

The Legendre transform of  $y \mapsto \eta(y)$  is defined implicitly for every  $z$  in the range of  $\eta_y$  by the relations

$$\eta(y) + \eta^*(z) = yz, \quad z = \eta_y(y).$$

The strict convexity of  $\eta$  insures that the second equation above can be solved for  $y$  in terms of  $z$ , thus allowing the elimination of  $y$  from the first equation.

It is easy to verify the dual nature of this transformation by using implicit differentiation to check that  $y = \eta_z^*(z)$ ; it is then clear that the Legendre transform of  $\eta^*$  is again  $\eta$ .

## Characterization of Equilibria

Hence, characterization (iii) is equivalent to

$$f = \eta_z^*(\beta \mathbf{e}), \quad \text{for some } \beta \in \mathbb{R}^{N^*}.$$

This formula will yield an equilibrium for every  $\beta$  in the set  $\mathbf{R}^*$  defined by

$$\mathbf{R}^* = \left\{ \beta \in \mathbb{R}^{N^*} : \eta_z^*(\beta \mathbf{e}) \in \text{Dom}(\mathcal{C}) \right\}.$$

The family of equilibria clearly depends only on  $\mathbb{E}$ ,  $\eta$ , and  $\text{Dom}(\mathcal{C})$ , and is completely independent of all other details of the collision operator.

### Example: Maxwellians

For kinetic theories where the entropy is  $\eta(f) = f \log(f) - f$ , the corresponding Legendre transform is  $\eta^*(z) = \exp(z)$ , and the equilibria given by  $f = \exp(\beta e)$ . When

$$e = \left(1, v_1, v_2, \dots, v_D, \frac{1}{2}|v|^2\right)^T,$$

then  $\exp(\beta e) = \mathcal{M}(\rho, u, \theta)$  where

$$\beta = \left( \log\left(\frac{\rho}{(2\pi\theta)^{D/2}}\right) - \frac{|u|^2}{2\theta}, \frac{u_1}{\theta}, \frac{u_2}{\theta}, \dots, \frac{u_D}{\theta}, -\frac{1}{\theta} \right),$$
$$\mathcal{M}(\rho, u, \theta) = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left(-\frac{|v-u|^2}{2\theta}\right).$$

Hence, the classical Maxwellians are recovered.

## The Density Potential

The formula for  $\mathcal{E}(\rho)$  can best be expressed through the introduction of the function  $h^*(\beta)$  defined over  $\mathbf{R}^*$  by

$$h^*(\beta) \equiv \langle \eta^*(\beta \mathbf{e}) \rangle .$$

The function  $h^*$  is strictly convex with Hessian

$$h_{\beta\beta^T}^*(\beta) = \langle \eta_{zz}^*(\beta \mathbf{e}) \mathbf{e} \mathbf{e}^T \rangle .$$

It is called the *density potential* because when it is differentiated with respect to  $\beta$  one finds that

$$\beta \mapsto \rho \equiv \langle \mathbf{e} \eta_z^*(\beta \mathbf{e}) \rangle = h_{\beta}^*(\beta) .$$

The range of this mapping is the set  $\mathbf{R}$ . The function  $h^*$  is therefore strictly convex, so this mapping is one-to-one from  $\mathbf{R}^*$  onto  $\mathbf{R}$ .

## Formula for Equilibria

The inverse mapping is then given by

$$\rho \mapsto \beta = h_\rho(\rho).$$

where  $h$  is the Legendre transform of  $h^*$ , which is defined implicitly for every  $\rho \in \mathbf{R}$  by

$$h(\rho) + h^*(\beta) = \beta\rho.$$

One thereby has that

$$\mathcal{E}(\rho) = \eta_z^*(h_\rho(\rho)\mathbf{e}) \quad \text{for every } \rho \in \mathbf{R}.$$

## Entropy Relations

The function  $h$  is the kinetic entropy density  $\langle \eta(f) \rangle$  restricted to the family of local equilibria,  $f = \mathcal{E}(\rho)$ , so that

$$h(\rho) = \langle \eta(\mathcal{E}(\rho)) \rangle.$$

Moreover, for every  $\rho \in \mathbf{R}$  one can show that

$$h(\rho) = \min \left\{ \langle \eta(f) \rangle : f \in \text{Dom}(\mathcal{C}), \langle \mathbf{e} f \rangle = \rho \right\}.$$

In other words, the kinetic entropy density  $\langle \eta(f) \rangle$  attains this constrained minimum at  $f = \mathcal{E}(\rho)$ .

## IV. GENERAL COMPRESSIBLE EULER SYSTEMS

A fluid description of the gas is valid when the Knudsen number is small. Set  $St = 1$  and  $Kn = \epsilon$ . The kinetic equation becomes

$$\partial_t F + v \cdot \nabla_x F = \frac{1}{\epsilon} \mathcal{C}(F).$$

The compressible Euler system is obtained by formally restricting  $F$  to the family of local equilibria. If we set  $F = \eta_z^*(\beta e)$  then the unknowns  $\beta = \beta(x, t)$  are governed by

$$\partial_t \langle e \eta_z^*(\beta e) \rangle + \nabla_x \cdot \langle v e \eta_z^*(\beta e) \rangle = 0.$$

Notice that the form of these equations depends only on the locally conserved quantities spanned by  $e$  and the velocities  $v$ .

## Potential Formulation

The Euler system can be recast in terms of the density potential  $h^*$  and the flux potential  $j^*$  defined by

$$h^*(\boldsymbol{\beta}) = \langle \eta^*(\boldsymbol{\beta}\mathbf{e}) \rangle, \quad j^*(\boldsymbol{\beta}) \equiv \langle v \eta^*(\boldsymbol{\beta}\mathbf{e}) \rangle.$$

Differentiating  $h^*$  and  $j^*$  with respect to  $\boldsymbol{\beta}$  yields

$$h_{\boldsymbol{\beta}}^*(\boldsymbol{\beta}) = \langle \mathbf{e} \eta_z^*(\boldsymbol{\beta}\mathbf{e}) \rangle, \quad j_{\boldsymbol{\beta}}^*(\boldsymbol{\beta}) = \langle v \mathbf{e} \eta_z^*(\boldsymbol{\beta}\mathbf{e}) \rangle,$$

where the right-hand sides are just the density and flux of the Euler system. The Euler system can therefore be put into the so-called Godunov potential form as

$$\partial_t h_{\boldsymbol{\beta}}^*(\boldsymbol{\beta}) + \nabla_x \cdot j_{\boldsymbol{\beta}}^*(\boldsymbol{\beta}) = 0.$$

## Consequences of the Potential Formulation

First, the hyperbolicity of the Euler system is seen by rewriting it as

$$h_{\beta\beta^T}^*(\beta)\partial_t\beta^T + j_{\beta\beta^T}^*(\beta) \cdot \nabla_x\beta^T = 0.$$

Because  $h_{\beta\beta^T}^*$  is positive definite while  $j_{\beta\beta^T}^*$  is symmetric, this has the form of a symmetric hyperbolic system.

Second, upon multiplying the above on the left by  $\beta$  and integrating, the Euler system is seen to possess the additional local conservation law

$$\partial_t\left(\beta h_{\beta}^*(\beta) - h^*(\beta)\right) + \nabla_x \cdot \left(\beta j_{\beta}^*(\beta) - j^*(\beta)\right) = 0.$$

This what one obtains by setting  $F = \eta_z^*(\beta e)$  directly into the local entropy dissipation law.

## Density Formulation

The Euler system can be reformulated in terms of  $\rho = \rho(x, t)$  as

$$\partial_t \rho + \nabla_x \cdot j_{\beta}^*(h_{\rho}(\rho)) = 0.$$

Reformulated in terms of  $\rho$  the entropy equation becomes

$$\partial_t h(\rho) + \nabla_x \cdot j(\rho) = 0,$$

where the entropy flux  $j = j(\rho)$  is given by

$$j(\rho) = h_{\rho}(\rho) j_{\beta}^*(h_{\rho}(\rho)) - j^*(h_{\rho}(\rho)).$$

These can be obtained either by expressing  $\beta$  in terms of  $\rho$  in the potential formulation, or by setting  $F = \mathcal{E}(\rho)$  in the conservation and dissipation laws.

The Euler system is therefore symmetrizable in the sense of Friedrichs and Lax. This was shown to be equivalent to the existence of a Godunov potential form by Mock.

## Characteristic Velocities

The characteristic velocities of the Euler system associated with any wave vector  $k \in \mathbb{R}^D$  are the eigenvalues of the matrix  $k \cdot j_{\beta\beta^T}^*(\beta)$  with respect to the matrix  $h_{\beta\beta^T}^*(\beta)$ . They may be ordered as

$$\lambda_1 \leq \cdots \leq \lambda_n \leq \lambda_{n+1} \leq \cdots \leq \lambda_N,$$

where  $\lambda_n$  is given by the classical min-max characterization

$$\lambda_n = \min \left\{ \max_{\gamma \in \mathbf{B}} \left\{ \frac{\langle (\gamma \mathbf{e})^2 (k \cdot v) \eta_{zz}^*(\beta \mathbf{e}) \rangle}{\langle (\gamma \mathbf{e})^2 \eta_{zz}^*(\beta \mathbf{e}) \rangle} \right\} : \mathbf{B} \in \text{Lin}^n(\mathbb{R}^{N^*}) \right\}.$$

Here  $\text{Lin}^n(V)$  denotes the set of all  $n$ -dimensional linear subspaces of a linear space  $V$ .

## V. EXAMPLES

Of course, the Boltzmann equation described in the first lecture is in this general class of kinetic theories. More generally, its collision operator has the form

$$\mathcal{B}(f, f) = \iint (f'_* f' - f_* f) b(\omega, v_* - v) d\omega dv_*,$$

the collision kernel  $b$  has the classical form

$$b(\omega, v_* - v) = |v_* - v| \Sigma(|\omega \cdot n|, |v_* - v|), \quad n = \frac{v_* - v}{|v_* - v|},$$

where  $\Sigma \geq 0$  is the specific differential cross-section, which has units of area (length <sup>$D-1$</sup> ) over mass. The Boltzmann equation is in this general class of kinetic theories provided  $b$  satisfies certain mild technical conditions.

## Boltzmann Collision Kernels -1

In the case when the molecules are classical point particles of mass  $m$  that interact through a repulsive power-law potential of the form  $c/r^k$  then  $b$  has the factored form

$$b(\omega, v_* - v) = \hat{b}(|\omega \cdot n|) |v_* - v|^\beta, \quad \text{with} \quad \beta = 1 - 2\frac{D-1}{k}.$$

This will be locally integrable with respect to  $dv_*$  provided  $\beta > -D$ , which leads to the constraint

$$k > 2\frac{D-1}{D+1}.$$

When  $D = 3$  this becomes  $k > 1$ , which means the marginal case is the Coulomb potential  $c/r$ .

## Boltzmann Collision Kernels - 2

We will not give the function  $\hat{b}$  here. We will however remark that  $\hat{b}$  is well-behaved except for a singularity at  $\omega \cdot n = 0$  of the form

$$\hat{b}(|\omega \cdot n|) \sim |\omega \cdot n|^{-\hat{\beta}} \quad \text{as } \omega \cdot n \rightarrow 0, \quad \text{with } \hat{\beta} = 1 + \frac{D-1}{k}.$$

This singularity arises due to the infinite range of the  $c/r^k$  potential. It reflects the fact that there are many collisions in which the colliding molecules do not pass very close to each other and are therefore deflected only slightly. This singularity has proved difficult to analyze. For example, the fact that this singularity is not integrable with respect to  $d\omega$  means that  $\mathcal{B}^+(f, f)$  and  $\mathcal{B}^-(f, f)$  do not make sense. So-called cut-off collision kernels have therefore been introduced. These replace the exact  $\hat{b}$  above with a more benign one.

## Boltzmann-Like Kinetic Theories

Much of the structure developed in the first lecture for the Boltzmann equation is shared by many so-called Boltzmann-like kinetic theories. For this class of kinetic theories  $S = \mathbb{R}^D$  and  $d\sigma(v) = dv$ , so that the kinetic density is  $F(v, x, t)$  and the governing kinetic equation takes the form

$$\partial_t F + v \cdot \nabla_x F = \mathcal{C}(F).$$

The basis for conserved quantities is

$$\mathbb{E} = \text{span}\{1, v_1, v_2, \dots, v_D, |v|^2\},$$

and  $\eta(f) = f \log(f) - f$ .

## The BGK Operator

The simplest example of a classical collision operator is the so-called BGK collision operator introduced by Bhatnagar, Gross, and Krook. It is a simple relaxation model given by

$$\mathcal{C}_{BGK}(f) = \frac{1}{\tau(\rho, \theta)} (\mathcal{M}(\rho, u, \theta) - f),$$

where  $\mathcal{M}(\rho, u, \theta)$  is the local Maxwellian determined by the mass density  $\rho$ , bulk velocity  $u$ , and temperature  $\theta$ . The relaxation time  $\tau$  is a function such that  $\tau(\rho, \theta) > 0$  when  $\rho > 0$  and  $\theta > 0$ .

## The Fokker-Planck-Landau Operator

Another example of a classical collision operator is the Fokker-Planck-Landau operator, which is representative of the larger class of Fokker-Planck operators. It models the effect of collisions as a diffusion in velocity. This kind of approximation is appropriate when most collisions produce small deflections in the velocities of the molecules involved. The Fokker-Planck-Landau operator has the form

$$\mathcal{C}_{FPL}(f) = \nabla_v \cdot \left[ \varsigma(\rho, \theta) \int \frac{|w|^2 I - w \otimes w}{|w|^3} (f_* \nabla_v f - f \nabla_{v_*} f_*) dv_* \right].$$

where  $w = v_* - v$  and the coefficient  $\varsigma$  is a function such that  $\varsigma(\rho, \theta) > 0$  when  $\rho > 0$  and  $\theta > 0$ .

## Generalized BGK Operators

Given any strictly convex  $\eta$  and any space  $\mathbb{E}$  there exist a collision operator  $\mathcal{C}$  which has  $\mathbb{E}$  as the locally conserved quantities, and which satisfies the entropy dissipation properties:

$$\mathcal{C}(f) = \frac{1}{\tau(\rho)} \left( \mathcal{E}(\rho) - f \right), \quad \text{where } \rho = \langle \mathbf{e} f \rangle.$$

This model generalizes the classical BGK relaxation model for the collision operator, which corresponds to  $\eta(f) = f \log(f) - f$  and  $\mathbb{E} = \text{span}\{1, v_1, v_2, \dots, v_D, |v|^2\}$ . Here  $\tau(\rho) > 0$  is understood as a relaxation time.

## Kinetic Theories from Quantum Mechanics - 1

Classical particles obey Maxwell-Boltzmann statistics, which lies behind the classical entropy function,  $\eta(f) = f \log(f) - f$ . Quantum particles obey either Fermi-Dirac or Bose-Einstein statistics. The corresponding entropies are respectively

$$\eta_{FD}(f) = f \log(f) + (1 - f) \log(1 - f),$$
$$\eta_{BE}(f) = f \log(f) - (1 + f) \log(1 + f).$$

The associated Legendre duals are

$$\eta_{FD}^*(z) = \log(1 + e^z), \quad \eta_{BE}^*(z) = -\log(1 - e^z),$$

whereby the associated equilibria have the form

$$f = \partial_z \eta_{FD}^*(\beta e) = \frac{1}{1 + \exp(-\beta e)}, \quad f = \partial_z \eta_{BE}^*(\beta e) = \frac{1}{\exp(-\beta e) - 1}.$$

## Kinetic Theories from Quantum Mechanics - 2

When one considers only the contribution of binary collisions, the classical Boltzmann collision operator can be modified to be consistent with either Fermi-Dirac or Bose-Einstein statistics as

$$C_{FD}(f) = \iint \left( f'_* f' (1 - f_*) (1 - f) - f_* f (1 - f'_*) (1 - f') \right) b d\omega d\sigma(v_*),$$

$$C_{BE}(f) = \iint \left( f'_* f' (1 + f_*) (1 + f) - f_* f (1 + f'_*) (1 + f') \right) b d\omega d\sigma(v_*).$$

Motivated by the Uncertainty Principle, microscopic quantum states are counted by the non-dimensional phase-space measure  $m^D dv dx / \hbar^D$ , where  $\hbar$  is Planck's constant divided by  $2\pi$ . The kinetic densities are defined with respect to this measure, whereby  $d\sigma(v) = m^D dv / \hbar^D$

## Polyatomic Kinetic Theories - 1

Here we present a class of such models with  $s = (e, v) \in S = \mathbb{R}_+ \times \mathbb{R}^D$  and  $d\sigma(e, v) = J(e)de dv$ . Here  $v$  is the velocity of the center of mass of a molecule,  $me$  is the energy in all the internal modes of a molecule of mass  $m$ , and  $J(e)$  is a nonnegative density of states that will be specified below. The total energy of a molecule in the state  $(e, v, x)$  is thereby  $\frac{1}{2}m|v|^2 + me$ . The kinetic density is  $F(e, v, x, t)$  and the governing kinetic equation takes the form

$$\partial_t F + v \cdot \nabla_x F = \mathcal{C}(F).$$

Here a basis for the conserved quantities is

$$\mathbb{E} = \text{span}\left\{1, v_1, v_2, \dots, v_D, \frac{1}{2}|v|^2 + e\right\},$$

and the entropy is again  $\eta(f) = f \log(f) - f$ .

## Polyatomic Kinetic Theories - 2

Suppose the dynamics of an individual molecule that is free from interactions with other molecules is governed by the classical Hamiltonian system

$$\frac{dp}{dt} = -H_q(p, q), \quad \frac{dq}{dt} = H_p(p, q),$$

where  $H(p, q)$  is the single-molecule Hamiltonian. The variable  $q$  specifies the configuration of the atoms in the molecule while the variable  $p$  specifies the associated momentum.

When  $(p, q)$  satisfies this system the evolution of any quantity  $G(p, q)$  is given by

$$\frac{dG}{dt} = H_p \cdot G_q - H_q \cdot G_p \equiv \{G, H\},$$

where  $\{ \cdot, \cdot \}$  defined above is called the Poisson bracket.

### Polyatomic Kinetic Theories - 3

Let the center of mass of the molecule be given by  $R(q)$ . The velocity of the center of mass is then given by  $V(p, q) = \{R, H\}(p, q)$ . This is conserved by the dynamics, so that  $\{V, H\} = 0$ . The Hamiltonian then has the form

$$H(p, q) = \frac{1}{2}m|V(p, q)|^2 + mI(p, q),$$

where  $mI(p, q)$  is the energy in all the internal modes of the molecule. The density of states  $J(e)$  can then be expressed as

$$J(e) = \iint \delta(e - I) \delta(v - V) \delta(x - R) dp dq,$$

where  $\delta(\cdot)$  denotes the Dirac delta function. We assume that the molecular dynamics respects Galilean symmetry. The fact that  $J$  is independent of  $x$  and  $v$  follows from this Galilean symmetry.

## Polyatomic Kinetic Theories - 4

The local equilibria for the polyatomic kinetic equation have the form  $f = \mathcal{M}_J(\rho, u, \theta)$  where

$$\mathcal{M}_J(\rho, u, \theta)(e, v) = \frac{\rho}{(2\pi\theta)^{D/2} Z(\theta)} \exp\left(-\frac{\frac{1}{2}|v-u|^2 + e}{\theta}\right),$$

for some  $\rho \geq 0$ ,  $u \in \mathbb{R}^D$ , and  $\theta > 0$ . Here  $Z(\theta)$  is defined by

$$Z(\theta) = \int_0^\infty \exp\left(-\frac{e}{\theta}\right) J(e) de,$$

while  $(\rho, u, \theta)$  are determined from  $f$  through the relations

$$\langle f \rangle = \rho, \quad \langle v f \rangle = \rho u, \quad \langle (\frac{1}{2}|v|^2 + e) f \rangle = \frac{1}{2}\rho|u|^2 + \rho\varepsilon(\theta),$$

where  $\varepsilon(\theta)$  is the specific internal energy which is given by

$$\varepsilon(\theta) = \frac{D}{2}\theta + \theta^2 \partial_\theta \log(Z(\theta)).$$

## Polyatomic Kinetic Theories - 5

We remark that the last term in

$$\varepsilon(\theta) = \frac{D}{2}\theta + \theta^2 \partial_\theta \log(Z(\theta))$$

gives the average specific energy in all the internal modes of molecules. It is an increasing function of  $\theta$ .

The corresponding compressible Euler system has the form

$$\begin{aligned} \partial_t \rho + \nabla_x \cdot (\rho u) &= 0, \\ \partial_t(\rho u) + \nabla_x \cdot (\rho u \otimes u) + \nabla_x(\rho \theta) &= 0, \\ \partial_t \left( \rho \left( \frac{1}{2} |u|^2 + \varepsilon(\theta) \right) \right) + \nabla_x \cdot \left( \rho u \left( \frac{1}{2} |u|^2 + \varepsilon(\theta) + \theta \right) \right) &= 0. \end{aligned}$$

This system of  $D+2$  equations for the  $D+2$  unknowns  $\{\rho, u_1, u_2, \dots, u_D, \theta\}$  is therefore closed. This is the compressible Euler system for an ideal gas.

## Polyatomic Kinetic Theories - 6

Perhaps you recall from thermodynamics that the pressure  $p$  of an ideal is given by the famous ideal gas law,  $p = \rho\theta$ , while the specific internal energy is an increasing function of  $\theta$  that is independent of  $\rho$ . The special case of a  $\gamma$ -law polytropic gas is recovered when

$$J(e) = \frac{k e^{\alpha-1}}{\Gamma(\alpha)} \quad \text{for some } \alpha > 0 \text{ and } k > 0,$$

where  $\Gamma(\cdot)$  is the classical Gamma function. One then finds that

$$Z(\theta) = k \theta^\alpha, \quad \varepsilon(\theta) = \left(\frac{D}{2} + \alpha\right)\theta,$$

from which one sees the “ $\gamma$ ” of this gas is given by

$$\gamma = 1 + \frac{2}{D + 2\alpha}.$$

The “dumbbell” model of a diatomic molecule yields  $\alpha = \frac{D-1}{2}$ .