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Extended thermodynamics---a theory of symmetric hyperbolic field equations

Applications of Mathematics, Vol. 53 (2008), No. 5, 469--484

Persistent URL: `http://dml.cz/dmlcz/140335`

EXTENDED THERMODYNAMICS—A THEORY OF SYMMETRIC HYPERBOLIC FIELD EQUATIONS

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Dedicated to Jürgen Sprekels on the occasion of his 60th birthday

Abstract. Extended thermodynamics is based on a set of equations of balance which are supplemented by local and instantaneous constitutive equations so that the field equations are quasi-linear differential equations of first order. If the constitutive functions are subject to the requirements of the entropy principle, one may write them in symmetric hyperbolic form by a suitable choice of fields.

The kinetic theory of gases, or the moment theories based on the Boltzmann equation, provide an explicit example for extended thermodynamics. The theory proves its usefulness and practicality in the successful treatment of light scattering in rarefied gases.

It would seem that extended thermodynamics is worthy of the attention of mathematicians. It may offer them a non-trivial field of study concerning hyperbolic equations, if ever they get tired of the Burgers equation.

Keywords: thermodynamics, symmetric hyperbolicity, kinetic theory, light scattering

MSC 2010: 80A17

1. Formal structure[1]

The objective of extended thermodynamics is the determination of n fields, synthetically denoted by $u_\alpha(x^d, t)$ $(\alpha = 1, 2, \ldots, n)$, and called densities. The argument x^d denotes the spatial coordinates of an event and t is its time. Invariably the first five of these fields are chosen as the densities of mass, momentum, and energy—and that is all in ordinary thermodynamics. But in extended thermodynamics the number of fields is extended (*sic*!) and it may contain the stress, the heat flux and more, see below.

[1] This presentation is based upon the book [15] of which the author of this paper is a co-author. For more details on motivation and exploitation of the basic principles the interested reader is referred to that book.

For the determination of the fields $u_\alpha(x^d, t)$ we need n field equations, and these are based upon n equations of balance[2]

$$\frac{\partial u_\alpha}{\partial t} + \frac{\partial F_\alpha^d}{\partial x^d} = \Pi_\alpha \quad (\alpha = 1, 2, \ldots, n). \tag{1.1}$$

The quantities F_α^d $(d = 1, 2, 3)$ are called fluxes and Π_α are called productions.

If the first five equations of (1.1) represent the conservation laws of mass, momentum, and energy, the first five productions Π_α $(\alpha = 1, \ldots, 5)$ vanish. And *all* productions vanish in an equilibrium.

In order to obtain field equations for the densities u_α, the equations of balance must be supplemented by constitutive equations. Such constitutive equations relate the fluxes and productions to the densities in a manner characteristic for the material. In extended thermodynamics the constitutive relations have the forms

$$F_\alpha^d = \hat{F}_\alpha^d(u_\beta) \quad \text{and} \quad \Pi_\alpha = \hat{\Pi}_\alpha(u_\beta), \tag{1.2}$$

so that the fluxes F_α^d and productions Π_α at a point and a time depend only on the densities at that point and time. We may say that the constitutive equations are local in space-time.[3]

If the constitutive functions $\hat{F}_\alpha^d$ and $\hat{\Pi}_\alpha$ were known explicitly, we could eliminate F_α^d and Π_α between the equations of balance and the constitutive relations and obtain explicit field equations for the u_α's. They form a quasi-linear system of partial differential equations of first order. Every solution of this system is called a *thermodynamic process.*

2. Symmetric hyperbolic systems

In reality, of course, the constitutive functions are not known, and it is the task of the constitutive theory to determine those functions or, at least, to reduce their generality. The tools of the constitutive theory are certain universal physical principles which represent expectations based on experience. The main principles are

- the entropy inequality,
- the requirement of concavity,
- the principle of relativity.

The first two of these combined represent the entropy principle.

[2] Summation is implied over repeated indices, whether Greek or Latin.

[3] Thus no gradients or time derivatives occur among the variables in the constitutive equations. In particular, there is no temperature gradient. And yet, heat conduction is accounted for, because the heat flux is counted among the variables.

The entropy inequality is an additional balance law which we write as

$$\frac{\partial h}{\partial t} + \frac{\partial h^d}{\partial x^d} = \Sigma \geqslant 0 \quad \text{for all thermodynamic processes.} \tag{2.1}$$

Here h is the entropy density and h^d is the entropy flux; Σ is the entropy production, assumed non-negative for all thermodynamic processes. All three of those quantities are constitutive quantities so that in extended thermodynamics we have

$$h = \hat{h}(u_\beta), \quad h^d = \hat{h}^d(u_\beta), \quad \Sigma = \hat{\Sigma}(u_\beta). \tag{2.2}$$

The requirement of concavity demands that h be a concave function of u_β, i.e.

$$\frac{\partial^2 h}{\partial u_\alpha \partial u_\beta} \text{ is negative definite.} \tag{2.3}$$

This makes it possible for the entropy to be maximal in equilibrium.

The principle of relativity states that the field equations and the entropy inequality have the same forms in all Galilei frames.[4]

We defer the consideration of the principle of relativity and proceed with the exploitation of the entropy principle. The key to the exploitation of the entropy inequality lies in the observation that the inequality need not hold for all fields u_α; rather it must hold for thermodynamic processes, i.e. solutions of the field equations. In a manner of speaking the field equations provide constraints for the fields that must satisfy the entropy inequality. A lemma by Liu [10] proves that it is possible to use Lagrange multipliers Λ_β—functions of u_α—to eliminate the constraints. Indeed, the new inequality

$$\frac{\partial h}{\partial t} + \frac{\partial h^d}{\partial x^d} - \Lambda_\alpha \Big(\frac{\partial u_\alpha}{\partial t} + \frac{\partial F^d_\alpha}{\partial x^d} - \Pi_\alpha \Big) \geqslant 0$$

must hold for all fields $u_\alpha(x^d, t)$. In particular this inequality must hold for arbitrary derivatives $\partial u_\alpha / \partial t$ and $\partial u_\alpha / \partial x^d$ at one event, and this implies

$$\mathrm{d}h = \Lambda_\alpha \, \mathrm{d}u_\alpha, \quad \mathrm{d}h^d = \Lambda_\alpha \, \mathrm{d}F^d_\alpha, \quad \text{and} \quad \Lambda_\alpha \Sigma_\alpha \geqslant 0. \tag{2.4}$$

From $(2.4)_1$ we conclude that

$$\frac{\partial \Lambda_\alpha}{\partial u_\beta} = \frac{\partial^2 h}{\partial u_\alpha \partial u_\beta}$$

[4] In relativistic thermodynamics we require the same invariance under Lorentz transformations.

is negative definite because of the concavity of h as a function of u_α. Therefore there is a one-to-one correspondence between the densities u_α and the Lagrange multipliers Λ_β. It is thus possible to make a change of variables $u_\alpha \Leftrightarrow \Lambda_\alpha$. If this is done, the two equations $(2.4)_{1,2}$ may be written in the form

$$\mathrm{d}h' = u_\alpha \,\mathrm{d}\Lambda_\alpha, \quad \mathrm{d}h'^d = F_\alpha^d \,\mathrm{d}\Lambda_\alpha, \tag{2.5}$$

where $h' = -h + \Lambda_\alpha u_\alpha$ and $h'^a = -h^a + \Lambda_\alpha F_\alpha^a$ are called scalar and vector potentials respectively, because their derivatives with respect to Λ_α are the densities and the fluxes. Therefore in the new variables the system of field equations reads

$$\frac{\partial^2 h'}{\partial\Lambda_\alpha\partial\Lambda_\beta}\frac{\partial\Lambda_\beta}{\partial t} + \frac{\partial^2 h'^d}{\partial\Lambda_\alpha\partial\Lambda_\beta}\frac{\partial\Lambda_\beta}{\partial x^d} = \Pi_\alpha \quad (\alpha = 1, 2, \ldots, n). \tag{2.6}$$

All four matrices in this system are obviously symmetric and the first one is negative definite.[5] Therefore the system of field equations (written in terms of Lagrange multipliers) is a *symmetric hyperbolic system.*

Hyperbolicity guarantees finite speeds of propagation and *symmetric* hyperbolic systems have convenient and desirable mathematical properties, namely well-posedness of Cauchy problems, i.e. existence, uniqueness, and continuous dependence on the data. The desire for finite speeds of propagation was the primary original incentive for the formulation of extended thermodynamics by Müller [13].

The residual inequality $(2.4)_3$ is due entirely to the production terms in the field equations; recall that the first five productions are zero. Since Π_α may be considered as a function of the Lagrange multipliers Λ_β, it follows from the inequality that in the equilibrium defined by $\Pi_\alpha|_E = 0$ all Λ_β $(\beta = 6, 7, \ldots, n)$ are equal to zero,

$$\Lambda_\beta|_E = 0 \quad (\beta = 6, 7, \ldots, n). \tag{2.7}$$

The residual inequality is a sum of products of the productions and the Lagrange multipliers. In the jargon of ordinary (non-extended) thermodynamics we may consider these quantities as thermodynamic forces and fluxes. And in a linear theory the forces are linear functions of the fluxes, so that we may write

$$\Pi_\alpha = \sum_{\beta=6}^{n} L_{\alpha\beta}\Lambda_\beta \quad (\alpha = 6, 7, \ldots, n). \tag{2.8}$$

[5] This follows from the concavity of the entropy density in terms of the densities u_α, since $h' = -h + \Lambda_\alpha u_\alpha$ defines a Legendre transformation associated to the map $u_\alpha \Leftrightarrow \Lambda_\alpha$. Such a Legendre transformation preserves concavity so that h' is a concave function of Λ_α.

3. Characteristic speeds and pulse speed

A wave is a moving surface, represented mathematically by the equation

$$\varphi(x^d, t) = 0,$$

which defines the wave front. The unit normal n^d and the normal speed V are given by

$$n^d = \frac{\partial\varphi/\partial x^d}{|\operatorname{grad}\varphi|} \quad \text{and} \quad V = -\frac{\partial\varphi/\partial t}{|\operatorname{grad}\varphi|}. \tag{3.1}$$

In the simple case considered here the wave front separates the constant and homogeneous fields $\Lambda_\alpha(x^d, t)$ in front of the wave from the perturbed fields behind it. In the case of weak waves, or acceleration waves[6], the fields are continuous across the front, but the gradients have a jump and, obviously, that jump points in the direction of the normal. Therefore

$$[\Lambda_\alpha] = 0 \quad \text{and hence} \quad \Big[\frac{\partial\Lambda_\alpha}{\partial x^d}\Big] n^d = J_\alpha \quad \text{and} \quad \Big[\frac{\partial\Lambda_\alpha}{\partial t}\Big] = -V J_\alpha, \tag{3.2}$$

where a square bracket $[a]$ denotes the difference of a generic quantity a in front of the wave and behind it. Here J_α ($\alpha = 1, 2, \ldots, n$) are called the *amplitudes* of the acceleration wave.

In our case the speeds and amplitudes are given by the field equations (2.6) as solutions of the homogeneous linear algebraic system

$$\Big(\frac{\partial^2 h'}{\partial\Lambda_\alpha\partial\Lambda_\beta} V - \frac{\partial^2 h'^d}{\partial\Lambda_\alpha\partial\Lambda_\beta} n^d\Big) J_\beta = 0. \tag{3.3}$$

Thus the possible wave speeds in the direction n^d are the solutions of the characteristic equation

$$\det\Big(\frac{\partial^2 h'}{\partial\Lambda_\alpha\partial\Lambda_\beta} V - \frac{\partial^2 h'^d}{\partial\Lambda_\alpha\partial\Lambda_\beta} n^d\Big) = 0. \tag{3.4}$$

We obtain n speeds and they are called *characteristic speeds*. The fastest one of these is called the *pulse speed*. All speeds are real and finite as a consequence of the symmetric hyperbolic character of the field equations.

By (3.3) the amplitudes J_β are right eigenvectors of the matrix of the linear system.

[6] In fluid mechanics weak waves have a continuous velocity across the front but a jump of acceleration; hence the name acceleration wave.

4. Growth and decay of acceleration waves

The solutions of non-linear hyperbolic equations have a tendency to develop singular derivatives even when the initial data are smooth. Thus jumps or shocks may appear. However, dissipation represented by the productions in the equations (2.6) can put a check on this tendency.

The conditions on initial data and on the dissipative terms which need to be satisfied to guarantee smooth solutions for all times are unknown. All we have is a sufficient condition for smoothness by Kawashima [9]. However, the treatment of acceleration waves gives a good intuitive understanding of what is involved.

It is possible to determine the rate of change $\partial J/\partial t$ of the amplitude of acceleration waves. This was first done by W. A. Green [8] but the most elegant derivation and result is due to Boillat [1]. We shall restrict the attention to the case that the wave propagates into a region of equilibrium with constant and homogeneous fields. In that case Boillat's result reduces to a Bernoulli equation with constant coefficients

$$\frac{\partial J}{\partial t} - \underbrace{\frac{\partial V}{\partial \Lambda_\beta} d_\beta}_{a} J^2 - \underbrace{l_\alpha \frac{\partial \Pi_\alpha}{\partial u_\beta} d_\beta}_{b} J = 0. \tag{4.1}$$

Here l_α and d_α are the left and the right eigen-values of the matrix of the linear system (3.3). The coefficient a, indicated in (4.1), represents the non-linearity of the system, namely the dependence of the wave speed upon the value of the fields Λ_α. The coefficient b represents dissipation, because it depends on the productions in the field equations.

The solution of (4.1) reads

$$J(t) = \frac{J(0)\mathrm{e}^{-bt}}{1 - J(0)ab^{-1}(\mathrm{e}^{-bt} - 1)}. \tag{4.2}$$

If the system were linear, i.e. $a = 0$, there would be exponential decay, of course. But even for $a \neq 0$ there may be decay unless the initial amplitude is too big. If that amplitude is big enough, $J(t)$ becomes singular at some time. For an acceleration wave this means that the amplitude of acceleration becomes infinite, so that the velocity has a jump; a shock wave appears, a discontinuity of velocity.

Experiments show that discontinuities do not exist. *Natura non fecit saltus!* If a mathematical theory predicts discontinuities, e.g. jumps of velocity in a shock wave, it is a sure sign that the theory is deficient and additional fields are required to resolve the discontinuity into a steep but smooth structure. Extended thermodynamics of moments shows the way in which this may be done, cf. [15]. Parabolisation of the field equations—euphemistically called regularization by mathematicians—is *not* the correct way.

5. An example. Extended thermodynamics of moments

5.1. Pulse speeds

The kinetic theory of gases is based on the Boltzmann equation for the distribution function $f(x^d, c^d, t)$ which determines the number density of atoms of the mass μ with the velocity c^d at the point x^d and time t. The moments of the distribution function are

$$u_{i_1 i_2 \ldots i_l} = \int \mu c_{i_1} c_{i_2} \ldots c_{i_l} f \,\mathrm{d}c, \tag{5.1}$$

so that u, u_i, and u_{ii} are the densities of mass, momentum and energy of the gas. The moments obey equations of balance of the form (1.1), *viz.*

$$\frac{\partial u_{i_1 i_2 \ldots i_l}}{\partial t} + \frac{\partial u_{i_1 i_2 \ldots i_l d}}{\partial x^d} = \Pi_{i_1 i_2 \ldots i_l} \quad (l = 0, 1, 2, \ldots, N). \tag{5.2}$$

For u, u_i, and u_{ii} the productions Π, Π_i, and Π_{ii} vanish because of the conservation of mass, momentum and energy in atomic collisions. Since each index may assume the values 1, 2, 3, there are $n = \frac{1}{6}(N+1)(N+2)(N+3)$ equations.

These equations fit into the formal framework of extended thermodynamics, but they are simpler.[7] Therefore the results of Sections 2 and 3 may be carried over to the present case, in particular the exploitation of the entropy inequality. In the kinetic theory of gases that inequality assumes the form[8]

$$\frac{\partial}{\partial t}\Big(-k \int f \ln \frac{f}{\mathrm{e}Y} \,\mathrm{d}c\Big) + \frac{\partial}{\partial x^a}\Big(-k \int c_a f \ln \frac{f}{\mathrm{e}Y} \,\mathrm{d}c\Big) \geqslant 0. \tag{5.3}$$

The exploitation makes use of the Lagrange multipliers $\Lambda_{i_1 i_2 \ldots i_l}$ $(l = 0, 1, 2, \ldots N)$ and the moment character of the densities and fluxes implies that the distribution function has the form

$$f = Y \exp\Big(-\frac{1}{k}\Lambda_{i_1 i_2 \ldots i_l} \mu c_{i_1} c_{i_2} \ldots c_{i_l}\Big), \tag{5.4}$$

so that the scalar and vector potential may be written as

$$h' = -kY \int \exp\Big(-\frac{1}{k}\Lambda_{i_1 i_2 \ldots i_l} \mu c_{i_1} c_{i_2} \ldots c_{i_l}\Big) \,\mathrm{d}c \tag{5.5}$$

and

$$h'^a = -kY \int c_a \exp\Big(-\frac{1}{k}\Lambda_{i_1 i_2 \ldots i_l} \mu c_{i_1} c_{i_2} \ldots c_{i_l}\Big) \,\mathrm{d}c.$$

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[7] Indeed, on the left-hand side there is only one flux, namely $u_{i_1 i_2 \ldots i_N d}$, the last one, which is not explicitly related to $u_{i_1 i_2 \ldots i_l}$ $(l = 0, 1, 2, \ldots, N)$.

[8] Here e is the Euler number and $1/Y$ is the smallest cell of the phase space spanned by x^a and c_a.

Insertion into the characteristic equation (3.4) for the calculation of the wave speeds gives

$$\det\left(\int (c_a n_a - V) c_{i_1} c_{i_2} \dots c_{i_l} f_E \,\mathrm{d}c\right) = 0 \tag{5.6}$$

provided that the wave propagates into a region of equilibrium. By f_E we denote the Maxwell distribution.

Thus the calculation of characteristic speeds and, in particular, the pulse speed, requires no more than simple quadratures and the solution of an nth order algebraic equation. It is true that the dimension of the determinant in (5.6) increases rapidly with N: For $N = 10$ we have 286 rows and columns, while for $N = 40$ we have 12341 of them. But then, the calculation of the elements of the determinant and the determination of the pulse speed $V_{\max}$ may be programmed into the computer and W. Weiss [19] has the values ready for any reasonable N at the touch of a button, cf. Fig. 5.1. We recognize from the figure that the pulse speed goes up with increasing N and it never stops. Indeed, according to Boillat & Ruggeri [3] there exists a lower bound for $V_{\max}$ which tends to infinity for $N \to \infty$.

N	n	$V_{\max}/\sqrt{\frac{5}{3}\frac{k}{\mu}T}$
10	286	4.018
20	1771	6.080
30	5456	7.663
40	12341	8.997

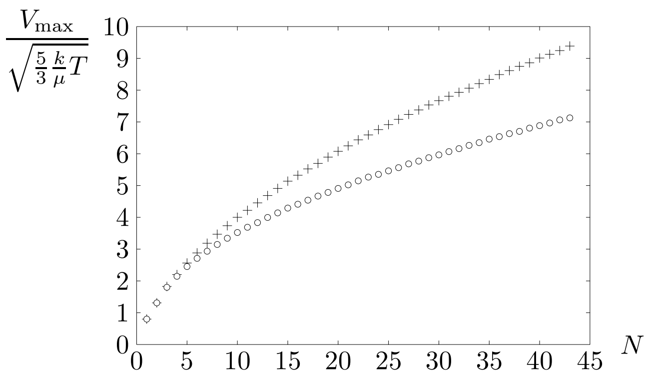

Figure 5.1. Pulse speeds referred to the normal sound speed. Table and crosses: Calculations by Weiss. Circles: Lower bound $\sqrt{\frac{6}{5}\left(N-\frac{1}{2}\right)}$ by Boillat and Ruggeri.

The fact that $V_{\max}$ is unbounded in a non-relativistic moment theory represents something of an anticlimax for extended thermodynamics, because that theory started out originally as an effort to find a *finite speed* of heat conduction. But it does not matter! Indeed by the time the conclusion was reached, extended thermodynamics had long outgrown its original motive.[9] It had become a predictive theory

[9] Anyway the problem lies with the kinetic theory rather than with extended thermodynamics. After all, infinite speeds of atoms are permitted in the non-relativistic kinetic theory and in the Maxwell distribution. For that reason the moments are integrals over the whole range of velocities from $-\infty$ to $+\infty$.

which is needed when steep gradients and rapid changes occur as they do in light scattering. Let us consider the situation in the following section.

5.2. Field equations for moments

Once the distribution function is known in terms of Lagrange multipliers, cf. (5.4), it is possible, in principle, to change back from the Lagrange multipliers $\Lambda_{i_1 i_2 \ldots i_l}$ to the moments $u_{i_1 i_2 \ldots i_l}$ by inverting the relation

$$u_{i_1 i_2 \ldots i_l} = \int \mu c_{i_1} c_{i_2} \ldots c_{i_l} Y \exp\Big(-\frac{1}{k}\, \Lambda_{i_1 i_2 \ldots i_l} \mu c_{i_1} c_{i_2} \ldots c_{i_l}\Big)\, \mathrm{d}c. \tag{5.7}$$

Once this is done, we may determine the last flux

$$u_{i_1 i_2 \ldots i_N d} = \int \mu c_{i_1} c_{i_2} \ldots c_{i_N} c_d Y \exp\Big(-\frac{1}{k}\, \Lambda_{i_1 i_2 \ldots i_l} \mu c_{i_1} c_{i_2} \ldots c_{i_l}\Big)\, \mathrm{d}c \tag{5.8}$$

in terms of the densities $u_{i_1 i_2 \ldots i_l}$ $(l = 0, 1, 2, \ldots, N)$. Also the productions may thus be calculated after we choose an appropriate model for the atomic interaction, e.g. the model of Maxwellian molecules.

In reality the calculations of the flux $u_{i_1 i_2 \ldots i_N d}$ and of the productions[10] $\Pi_{i_1 i_2 \ldots i_l}$ $(l = 6, 7, \ldots, N)$ require somewhat precarious approximations, since integrals of the type occurring in (5.8) cannot be solved analytically. Those approximations deserve further study[11] but when everything is said and done, one arrives at explicit field equations, e.g. those of Fig. 5.2, which are valid for $N = 3$ so that there are 20 individual equations. The equations written in the figure are linearized and the canonical notation has been introduced, like ϱ for the mass density u, ϱv_i for the momentum density u_i, $3/2\varrho k/\mu T$ for the energy density $1/2u_{ii}$, $t_{\langle ij\rangle}$ for the deviatoric stress and q_i for the heat flux. The moment $u_{\langle ijk\rangle}$ has no conventional name other than *trace-free third moment* because it does not enter the conventional equations of balance of mass, momentum, and energy. And yet, it does have to satisfy an explicit field equation.

The figure shows the same set of 20 equations four times so as to make it possible to point out special cases within the different frames.

- On the upper left side we see the equations for the Euler fluid, which is entirely free of dissipation and thus without shear stresses and heat flux.
- The upper right box contains the Navier-Stokes-Fourier equations with the stress proportional to the velocity gradient and the heat flux proportional to the temperature gradient. This set identifies the only unspecified coefficient τ as related

[10] Recall that the first five productions are zero because of the conservation of mass, momentum, and energy.
[11] A fully satisfactory theory of extended thermodynamics, which does not need the precarious approximation, is presented in [16].

$$\frac{\partial \varrho}{\partial t} + \overline{\varrho}\frac{\partial v_j}{\partial x_j} = 0$$

$$\frac{\partial v_i}{\partial t} + \frac{\frac{k}{\mu}\overline{T}}{\overline{\varrho}}\frac{\partial \varrho}{\partial x_j} + \frac{\partial \frac{k}{\mu}\overline{T}}{\partial x_i} - \frac{1}{\varrho}\frac{\partial t_{\langle ij\rangle}}{\partial x_j} = 0$$

$$\frac{\partial \frac{k}{\mu}T}{\partial T} + \frac{2}{3}\frac{k}{\mu}\overline{T}\frac{\partial v_k}{\partial x_k} + \frac{2}{3}\frac{1}{\overline{\varrho}}\frac{\partial q_k}{\partial x_k} = 0$$

$$\frac{\partial t_{\langle ij\rangle}}{\partial t} - \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} - \frac{\partial \varrho_{\langle ijk\rangle}}{\partial x_k} - 2\overline{\varrho}\frac{k}{\mu}\overline{T}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} = -\frac{3}{2}\frac{1}{\tau}t_{\langle ij\rangle}$$

$$\frac{\partial q_i}{\partial t} - \frac{k}{\mu}\overline{T}\frac{\partial t_{\langle ik\rangle}}{\partial x_k} + \frac{5}{2}\overline{\varrho}\frac{k}{\mu}\overline{T}\frac{\partial \frac{k}{\mu}T}{\partial x_i} = -\frac{1}{\tau}q_i$$

$$\frac{\partial \varrho_{\langle ijk\rangle}}{\partial t} - 3\frac{k}{\mu}\overline{T}\Big(\frac{\partial t_{(\langle ij\rangle}}{\partial x_{k)}} - \frac{2}{5}\frac{\partial t_{\langle r(i\rangle}}{\partial x_r}\delta_{jk)}\Big) = -\frac{9}{4}\frac{1}{\tau}\varrho_{\langle ijk\rangle}$$

$$\frac{\partial \varrho}{\partial t} + \overline{\varrho}\frac{\partial v_j}{\partial x_j} = 0$$

$$\frac{\partial v_i}{\partial t} + \frac{\frac{k}{\mu}\overline{T}}{\overline{\varrho}}\frac{\partial \varrho}{\partial x_j} + \frac{\partial \frac{k}{\mu}\overline{T}}{\partial x_i} - \frac{1}{\overline{\varrho}}\frac{\partial t_{\langle ij\rangle}}{\partial x_j} = 0$$

$$\frac{\partial \frac{k}{\mu}T}{\partial t} + \frac{2}{3}\frac{k}{\mu}\overline{T}\frac{\partial v_k}{\partial x_k} + \frac{2}{3}\frac{1}{\overline{\varrho}}\frac{\partial q_k}{\partial x_k} = 0$$

$$\frac{\partial t_{\langle ij\rangle}}{\partial t} - \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} - \frac{\partial \varrho_{\langle ijk\rangle}}{\partial x_k} - 2\overline{\varrho}\frac{k}{\mu}\overline{T}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} = -\frac{3}{2}\frac{1}{\tau}t_{\langle ij\rangle}$$

$$\frac{\partial q_i}{\partial t} - \frac{k}{\mu}\overline{T}\frac{\partial t_{\langle ik\rangle}}{\partial x_k} + \frac{5}{2}\overline{\varrho}\frac{k}{\mu}\overline{T}\frac{\partial \frac{k}{\mu}T}{\partial x_i} = -\frac{1}{\tau}q_i$$

$$\frac{\partial \varrho_{\langle ijk\rangle}}{\partial t} - 3\frac{k}{\mu}\overline{T}\Big(\frac{\partial t_{(\langle ij\rangle}}{\partial x_{k)}} - \frac{2}{5}\frac{\partial t_{\langle r(i\rangle}}{\partial x_r}\delta_{jk)}\Big) = -\frac{9}{4}\frac{1}{\tau}\varrho_{\langle ijk\rangle}$$

$$\frac{\partial \varrho}{\partial t} + \overline{\varrho}\frac{\partial v_j}{\partial x_j} = 0$$

$$\frac{\partial v_i}{\partial t} + = \frac{\frac{k}{\mu}\overline{T}}{\overline{\varrho}}\frac{\partial \varrho}{\partial x_j} + \frac{\partial \frac{k}{\mu}\overline{T}}{\partial x_i} - \frac{1}{\varrho}\frac{\partial t_{\langle ij\rangle}}{\partial x_j} = 0$$

$$\frac{\partial \frac{k}{\mu}T}{\partial t} + \frac{2}{3}\frac{k}{\mu}\overline{T}\frac{\partial v_k}{\partial x_k} + \frac{2}{3}\frac{1}{\overline{\varrho}}\frac{\partial q_k}{\partial x_k} = 0$$

$$\frac{\partial t_{\langle ij\rangle}}{\partial t} - \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} - \frac{\partial \varrho_{\langle ijk\rangle}}{\partial x_k} - 2\overline{\varrho}\frac{k}{\mu}\overline{T}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} = -\frac{3}{2}\frac{1}{\tau}t_{\langle ij\rangle}$$

$$\frac{\partial q_i}{\partial t} - \frac{k}{\mu}\overline{T}\frac{\partial t_{\langle ik\rangle}}{\partial x_k} + \frac{5}{2}\overline{\varrho}\frac{k}{\mu}\overline{T}\frac{\partial \frac{k}{\mu}T}{\partial x_i} = -\frac{1}{\tau}q_i$$

$$\frac{\partial \varrho_{\langle ijk\rangle}}{\partial t} - 3\frac{k}{\mu}\overline{T}\Big(\frac{\partial t_{(\langle ij\rangle}}{\partial x_{k)}} - \frac{2}{5}\frac{\partial t_{\langle r(i\rangle}}{\partial x_r}\delta_{jk)}\Big) = -\frac{9}{4}\frac{1}{\tau}\varrho_{\langle ijk\rangle}$$

$$\frac{\partial \varrho}{\partial t} + \overline{\varrho}\frac{\partial v_j}{\partial x_j} = 0$$

$$\frac{\partial v_i}{\partial t} + \frac{\frac{k}{\mu}\overline{T}}{\overline{\varrho}}\frac{\partial \varrho}{\partial x_j} + \frac{\partial \frac{k}{\mu}\overline{T}}{\partial x_i} - \frac{1}{\overline{\varrho}}\frac{\partial t_{\langle ij\rangle}}{\partial x_j} = 0$$

$$\frac{\partial \frac{k}{\mu}T}{\partial t} + \frac{2}{3}\frac{k}{\mu}\overline{T}\frac{\partial v_k}{\partial x_k} + \frac{2}{3}\frac{1}{\overline{\varrho}}\frac{\partial q_k}{\partial x_k} = 0$$

$$\frac{\partial t_{\langle ij\rangle}}{\partial t} - \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} - \frac{\partial \varrho_{\langle ijk\rangle}}{\partial x_k} - 2\overline{\varrho}\frac{k}{\mu}\overline{T}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} = -\frac{3}{2}\frac{1}{\tau}t_{\langle ij\rangle}$$

$$\frac{\partial q_i}{\partial t} - \frac{k}{\mu}\overline{T}\frac{\partial t_{\langle ik\rangle}}{\partial x_k} + \frac{5}{2}\overline{\varrho}\frac{k}{\mu}\overline{T}\frac{\partial \frac{k}{\mu}T}{\partial x_i} = -\frac{1}{\tau}q_i$$

$$\frac{\partial \varrho_{\langle ijk\rangle}}{\partial t} - 3\frac{k}{\mu}\overline{T}\Big(\frac{\partial t_{(\langle ij\rangle}}{\partial x_{k)}} - \frac{2}{5}\frac{\partial_{\langle r(i\rangle}}{\partial x_r}\delta_{jk)}\Big) = -\frac{9}{4}\frac{1}{\tau}\varrho_{\langle ijk\rangle}$$

Figure 5.2. Each one of the four groups represent the field equations of extended thermodynamics for $N = 3$. Top left: Euler equations. Top right: Navier-Stokes equations. Bottom left: Cattaneo equations. Bottom right: Grad's thirteen moment equations.

to the shear viscosity η. We have $\eta = \frac{4}{3}\tau\varrho\frac{k}{\mu}T$ so that η grows linearly with T as is expected for Maxwellian molecules.

- In the fifth equation of the third set I have highlighted the Cattaneo equation. Cattaneo [4] was a forerunner of extended thermodynamics, who provided a modification on the Fourier law on the grounds of kinetic arguments by adding a term with the rate of the heat flux to it.
- The fourth box exhibits the 13-moment equations. These were formulated by Grad [7] as an example for his moment method for the approximate determination of the consequences of the Boltzmann equation. They are the most popular equations of extended thermodynamics, because they contain only the moments ϱ, ϱv_i, T, $t_{\langle ij\rangle}$ and q_i known from ordinary thermodynamics.

For an interpretation we may rely on the upper right box in Fig. 5.2, the one that emphasizes the Navier-Stokes-Fourier theory. Inspection shows that some specific terms are left out of that theory, namely

$$\frac{\partial t_{\langle ij\rangle}}{\partial t} \quad \text{and} \quad \frac{\partial q_i}{\partial t} \quad \text{and} \quad \frac{\partial t_{\langle ij\rangle}}{\partial x^j} \quad \text{and} \quad \frac{\partial q_i}{\partial x^k}. \tag{5.9}$$

For rapid rates and steep gradients we may suspect that these terms *do* count and indeed they do, and we must go to the full set of 20 equations, or to equations with even more moments. Since the rapid rates and steep gradients are measured in terms of mean times of free flight and mean free paths, we may suspect that extended thermodynamics becomes necessary for rarefied gases.

5.3. Light scattering in gases as an example of extended thermodynamics of moments

The random thermal motion of the atoms or molecules of a gas disturbs the equilibrium of the gas and generates tiny and short lived compressions and expansions, i.e. fluctuations of density. These make the dielectric constant of the gas fluctuate, because it depends on the density. By Maxwell's equations the fluctuations cause a light wave to be scattered sideways, cf. Fig. 5.3 a). Most of the scattered light has the frequency $\omega^{(i)}$ of the incident mono-chromatic light, but neighbouring frequencies ω are also present in the scattering spectrum $S(\omega)$. Typically the *measured* spectrum—scattered in a gas and passed through an interferometer to a photomultiplier—exhibits three well-developed peaks, if the gas is normally dense. In a rarefied gas measurements show a flatter curve with lateral *shoulders*, cf. Fig. 5.3 b).

The light scattering spectrum may also be *calculated* from the field equations fort the gas, e.g. the Navier-Stokes-Fourier equations. The key to the calculation is the Onsager hypothesis by which the spatial Fourier components of the fields are the same functions of time as the mean regression of a fluctuation. For dense

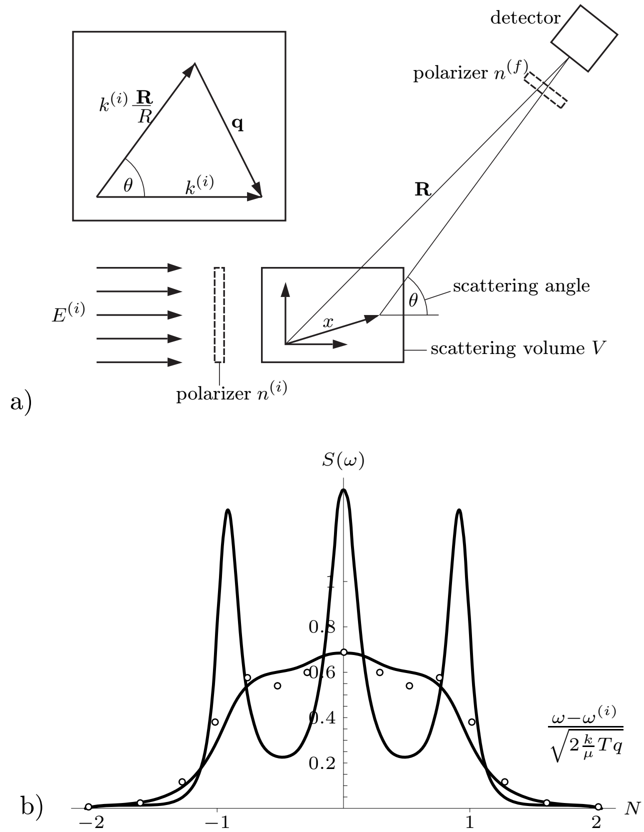

Figure 5.3. On light scattering. a) Light scattering, schematic. b) Scattering spectrum in a dense gas and in a rarefied gas. Dots: Measurements in a rarefied gas. Lines: Calculation by Navier-Stokes-Fourier theory.

gases the measured and calculated scattering spectra agree perfectly well. This fact supports the Onsager hypothesis. For a rarefied gas, however, the agreement is bad, cf. Fig. 5.3 b). Therefore we may conclude that the discrepancy is due to the Navier-Stokes-Fourier theory which, indeed, is expected to fail in a rarefied gas according to the considerations of Section 5.2.

So, this is a case where extended thermodynamics can prove its usefulness and practicality. Weiss [19] has applied the linearized field equations of 20, 35, 56, and 84 moments to the problem and has calculated the scattering spectra of Fig. 5.4 (top) for small pressures for which the experimental dots of Fig. 5.3 b were obtained. Inspection shows that the theories differ among themselves and that none of them fits the experimental points well. Nor can we adjust parameters to obtain a better fit, because there are no adjustable parameters of the usual type in extended thermodynamics. The only available parameter is the number of moments and moment equations. Therefore Weiss went ahead to 120 through 286 moments and obtained *convergence as well as a perfect fit*, cf. Fig. 5.4 (bottom).

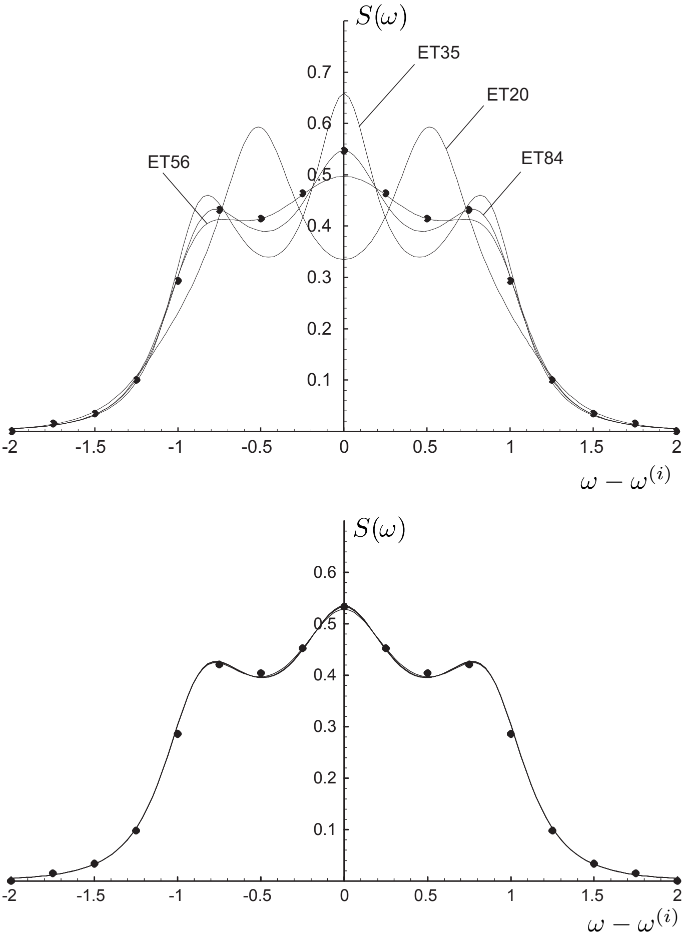

Figure 5.4. Light scattering spectra in a moderately rarefied gas. Dots represent measurements. Top: Extended thermodynamics of $N = 20, 35, 56, 84$ moments. Bottom: Extended thermodynamics of $N = 120, 165, 220, 286$.

That result might be called satisfactory, amazing and disappointing at the same time:

- Satisfaction comes from the fact that extended thermodynamics combined with the Onsager hypothesis is capable of representing light scattering satisfactorily in rarefied gases.

- The amazing feature is the convergence of the light scattering spectra at some finite number of moments. More moments will not appreciably change the calculated curves.
- Disappointment stems from the large number of moments needed to achieve convergence. We might have hoped that 13 or, perhaps 14 or 20 moments could give good results. That would have given us a manageable system of equations. Instead we need 120 of them—at least for the small pressures to which the curves of Fig. 5.4 refer.

And yet, the results for light scattering represent the claim to fame of extended thermo-dynamics. Indeed, the convergence put in evidence by the plots of Fig. 5.4 permits us to conclude that extended thermodynamics determines its own range of applicability without any reference to experiments. This is something that is often said to be impossible. Yet in extended thermodynamics it is possible because it is not a single theory; it is a *theory of theories*, one each for a given number of moments. So, if, after an increase of that number, we obtain the same function $S(\omega)$ in some norm, we have reached convergence and may fully trust the theory and predict the light spectrum, *without making a single experiment.*

6. On the origin and development of extended thermodynamics

When extended thermodynamics started with the work of Müller [13], [14] its sole and, from the present point of view, rather naive objective was the resolution of the so-called paradoxa of heat conduction and shear wave propagation: The Navier-Stokes-Fourier theory has a parabolic structure and it predicts infinite pulse speeds. Working within the then prevailing theory of **T**hermodynamics of **I**rreversible **P**rocesses (TIP), Müller allowed the local entropy to depend on the heat flux and the viscous stress. Also he assumed the entropy flux to be given by a generic constitutive equation rather than being determined universally by the ratio of heat flux and temperature, cf. [12]. This theory led to hyperbolic equations for temperature and shear velocities.

That early type of extended thermodynamics profited from the contact with the kinetic theory of gases—still in [14]—particularly with the moment method by Grad [7]. Later the connection between extended thermodynamics and the kinetic theory of gases became really close in the work [11] by Liu and Müller, where Lagrange multipliers were used for the exploitation of the entropy inequality. In this manner extended thermodynamics assumed a neat systematic form, albeit only for 13 or 14 moments.

Yet in this shape the theory was prepared to be joined to the mathematical theory of hyperbolic systems. Ruggeri and Strumia [18] recognized that the Lagrange multipliers—their *main field*—were privileged as a variable field and, if they are chosen, they make the field equations symmetric hyperbolic. With this observation it became possible to reveal the formal structure of extended thermodynamics which I have described in Sections 1 and 2 above. That formal structure applied to moments was refined and extended by Boillat and Ruggeri [17], [2]. In the end the authors proved in [3] that the pulse speed, though finite for any finite number of moments, tends to infinity for infinitely many moments, at least in the non-relativistic case.[12]

It seems that the significance of symmetric hyperbolic equations was first recognized by Godunov [6], who rewrote the conventional equations of fluid mechanics in symmetric hyperbolic form. Later Friedrichs and Lax [5] discovered that quasi-linear first order systems may be reduced to symmetric hyperbolic systems, if they are compatible with a "convex extension", i.e. an additional equation of balance type. Although widely quoted, the approach by Friedrichs and Lax is second best compared with the method of Ruggeri and Strumia [18]. Indeed, the eventual symmetric hyperbolic equations of Friedrichs and Lax are no longer equivalent to the original physically motivated balance laws and their solutions of shock structure problems, if they exist at all, are different from those of the original balance laws.

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