From Boltzmann to Euler: Hilbert's 6th problem revisited

Marshall Slemrod

Department of Mathematics
University of Wisconsin, Madison and Weizmann Institute of Sciences

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Outline

Hilbert 6th problem

In Hilbert's 1900 address to ICM in Paris, he proposed the problem for the limiting process which lead from the atomistic view to the laws of motion of continua. Passage from the kinetic Boltzmann equation for a rarefied gas to the continuum Euler equations of compressible gas dynamics as the Knudsen number $\varepsilon \to 0$.

As of this moment, success in the problem has been limited to cases where the limiting continuum equations possess smooth solutions, i.e. before shock formation. (An excellent up to date survey may be found in book of L. St. Raymond).

Is there an inherent mathematical reason that makes Hilbert's 6th problem unattainable and can we pinpoint this reason in a simple mathematical form ?.

The Chapman-Enskog expansion

- The Boltzmann equation:

$$\partial_t f + \xi \cdot \nabla f = \frac{Q(f, f)}{\varepsilon} \tag{1}$$

where $f = f(t, x, \xi)$ is the probability of finding a molecule of gas at point $x \in \mathbb{R}^3$, at time t, moving with velocity $\xi \in \mathbb{R}^3$. We note each ξ_i varies from $-\infty$ to ∞ and hence particles are allowed to have infinite velocities. The function f determines macroscopic fluid variables of density, momentum and temperature via its moments. Denote the density, momentum and temperature by ρ, $\rho\mathbf{u}$ and Θ. The Chapman–Enskog expansion is a formal power series in the Knudsen number $\varepsilon > 0$ for the function f in terms of these macroscopic varies (which we denote by M).

$$f_{CE}(M, \xi) = f^{(0)}(M, \xi) + \varepsilon f^{(1)}(M, \xi) + \varepsilon^2 f^{(2)}(M, \xi) + \dots \tag{2}$$

$f^{(0)}(M, \xi)$ is the usual local Maxwellian. Truncation at 0th order yields the balance laws of mass, momentum and energy for an elastic fluid, i.e. compressible gas dynamics of an ideal gas. Truncation at order ε yields the Navier–Stokes–Fourier equations, truncation at order ε^2 yields the Burnett equations. Truncation at order yields the super-Burnett equations and so forth. The success of the Chapman–Enskog expansion to deliver the well known Navier-Stokes-Fourier theory at order has motivated many to view the Navier–Stokes–Fourier theory as fundamental in computing shock structure. But as seen from a simple one dimensional analogy, this justification is questionable.

If one wishes to determine the shock structure for the scalar conservation law

$$u_t + uu_x = 0$$

by imposition of a viscous term one gets Burgers' equation:

$$u_t + uu_x = \varepsilon u_{xx}.$$

Look for travelling wave solutions of the Burgers' equation

$$u = u\Big(\frac{x - ct}{\varepsilon}\Big)$$

and recover the ordinary differential equation x

$$-cu' + uu' = u''.$$

Thus in any study of non-smooth solutions to our original scalar conservation laws via imposition of higher gradient terms we see there is no concept of small derivative terms, i.e. all terms are a priori the same magnitude.

The ε has been scaled out ! Hence any study of non-smooth hydrodynamics via a truncation of the Chapman–Enskog expansion, while convenient is an illegitimate use of the Boltzmann equation.

"VATICINIUM EX EVENTU"
(A pseudo-prophecy written after the event)
James Kugel, How to read the bible, (2007).

Nevertheless the Chapman–Enskog expansion is an appealing tool since it allows us to cast Hilbert's question in the language and tools of partial differential equations.

But if truncations of C-E are illegitimate for non-smooth solutions of the fluid equations that leaves us only one recourse, i.e. summation of the entire Champan-Enskog expansion. This is exactly what A. Gorban and I. Karlin have done in a remarkable series of papers.

Results of Gorban and Karlin

Take the first 13 moments of the Boltzmann equations and then close the system by Grad's closure rule for f.

• The Grad's 13 moment system linearized about the rest state:

$$
\begin{aligned}
\partial_t \rho &= -\nabla \cdot \mathbf{u}, \\
\partial_t \mathbf{u} &= -\nabla \rho - \nabla \Theta - \nabla \cdot \boldsymbol{\sigma}, \\
\partial_t \Theta &= -\frac{2}{3} \left(\nabla \cdot \mathbf{u} + \nabla \cdot \mathbf{q} \right), \\
\partial_t \sigma &= -\left((\nabla \mathbf{u}) + (\nabla \mathbf{u})^T - \frac{2}{3} \nabla \cdot \mathbf{u}\,\mathbf{I} \right) \\
&\quad -\frac{2}{3} \left((\nabla \mathbf{q}) + (\nabla \mathbf{q})^T - \frac{2}{3} \nabla \cdot \mathbf{q}\,\mathbf{I} \right) - \boldsymbol{\sigma}, \\
\partial_t \mathbf{q} &= -\frac{5}{3} \nabla \Theta - \nabla \cdot \boldsymbol{\sigma} - \frac{2}{3} \mathbf{q}, \\
p &= \rho + \Theta.
\end{aligned}
$$

• A simplified 10 moment theory in one space dimension:

$$
\begin{aligned}
\partial_t p &= -\frac{5}{3}\partial_x u, \\
\partial_t u &= -\partial_x p - \partial_x \sigma, \\
\partial_t \sigma &= -\frac{4}{3}\partial_x u - \frac{\sigma}{\varepsilon}.
\end{aligned}
$$

(Rescaled $x = x'/\varepsilon$, $t = t'/\varepsilon$ and then dropped the prime).

The role of the Knudsen number ε becomes apparent, i.e. it is an ordering tool for the Chapman–Enskog expansion. Write the C-E expansion

$$
\sigma_{CE} = \varepsilon\sigma^{(0)} + \varepsilon^2\sigma^{(1)} + \varepsilon^3\sigma^{(2)} + \ldots
$$

where $\sigma^{(n)}$ depend on p, u and their space derivatives.

$$
\sigma_{CE} = -\frac{4}{3}\left(\varepsilon\partial_x u + \varepsilon^2\partial_x p + \frac{\varepsilon^3}{3}\partial_x^3 u + \ldots\right).
$$

Truncation as orders $\varepsilon, \varepsilon^2, \varepsilon^3$, yields dispersion relations

• (Euler order):
$$\omega_\pm = -\frac{2}{3}k^2 \pm \frac{i|k|}{3}\sqrt{4k^2 - 15}.$$

• (Navier-Stokes order):
$$\omega_\pm = -\frac{2}{3}k^2 \pm \frac{i|k|}{3}\sqrt{8k^2 + 15}.$$

• (Burnett order):
$$\omega_\pm = -\frac{2}{9}k^2(k^2 - 3) \pm \frac{i|k|}{9}\sqrt{4k^6 - 24k^4 - 72k^2 - 135}.$$

• (Super-Burnett order): we have a Bobylev instability for $k^2 > 3$, k being the frequency in Fourier space.

The goal of Gorban and Karlin was summation, NOT truncation.

Take the Fourier transform of σ_{CE} and sum the series.

$$
\begin{aligned}
\hat{\sigma}_{CE} &= \sum_{n=0}^{\infty} -ika_n(-k^2)^n \hat{u} + \sum_{n=0}^{\infty} -k^2 b_n(-k^2)^n \hat{p} \\
&= -ikA(k^2)\hat{u} - k^2 B(k^2)\hat{p}
\end{aligned}
$$

where

$$
A(k^2) = \sum_{n=0}^{\infty} -ika_n(-k^2)^n, \quad B(k^2) = \sum_{n=0}^{\infty} b_n(-k^2)^n.
$$

The good fortune in this example is that the sums A and B are related via the formula

$$A = \frac{B}{1 - k^2 B},$$

and that if B is written as $C = k^2 B$, then C satisfies the fundamental cubic equation

$$-\frac{5}{3}(1 - C)^2\left(C + \frac{4}{5}\right) - \frac{C}{k^2} = 0. \tag{3}$$

Eq. (3) has one real and two complex roots. The real root is the one of interest to us and is negative for $k^2 > 0$, $C(0) = 0$, and monotone decreasing in k^2, with asymptotic limit $C \to -4/5$ as $k^2 \to \infty$.

Hence A, B are known functions $A, B < 0$ for $k^2 > 0$.

In Fourier space, the hydrodynamics becomes

$$
\begin{aligned}
\hat{p}_t &= \frac{5}{3} i k \hat{u}, \\
\hat{u}_t &= i k \hat{p} + i k (-i k A(k^2) \hat{u}(t, k) - k^2 B(k^2) \hat{p}),
\end{aligned}
$$

We set

$$
\hat{p}(t, k) = e^{\omega t} P(k), \hat{u}(t, k) = e^{\omega t} U(k).
$$

Then P and U satisfy

$$
\begin{bmatrix} -\omega & \dfrac{5}{3} i k \\[2mm] i k - i k^3 B & k^2 A - \omega \end{bmatrix} \begin{bmatrix} P \\[2mm] U \end{bmatrix} = \begin{bmatrix} 0 \\[2mm] 0 \end{bmatrix}.
$$

Set the determinant of the coefficient matrix to zero and find the dispersion relation (spectrum in Fourier space)

$$\omega^2 - \omega k^2 A + \frac{5}{3}(k^2 - k^4 B) = 0, \quad \text{i.e.,}$$

$$\omega = \frac{1}{2}\left(\frac{C}{1-C}\right) \pm |k|\left(\left(\frac{C}{1-C}\right)^2 \frac{1}{k^2} - \frac{20}{3}(1-C)\right)^{1/2}$$
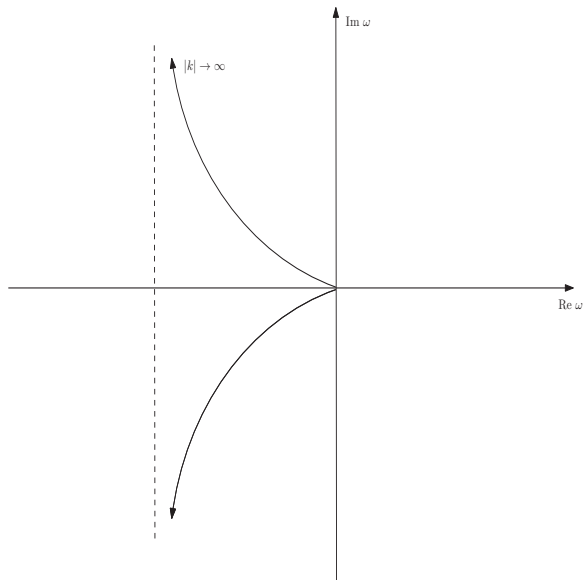
Recall C satisfies the cubic

$$-\frac{5}{3}(C-1)^2\left(C + \frac{4}{5}\right) = \frac{C}{k^2},$$

and hence $-\frac{5}{3}C\left(C + \frac{4}{5}\right) = \frac{C^2}{(1-C)^2}\frac{1}{k^2}$ and the formula for ω becomes

$$\omega = \frac{1}{2}\left(\frac{C}{C-1}\right) \pm i|k|\left(\frac{5C^2 - 16C + 20}{3}\right)^{1/2},$$

where we note that the quadratic form $5C^2 - 16C + 20$ is always positive. Since $C \to -\frac{4}{5}$ as $|k| \to \infty$ we see $Re\,\omega \to -\frac{2}{9}$ as $|k| \to \infty$

A sketch of the spectrum is given in Figure 1.

One issue not addressed by Gorban and Karlin in their papers was derivation of an entropy equality:

$$\frac{1}{2}\partial_t\left(\frac{3}{5}|\hat{\rho}|^2 + |\hat{u}|^2\right) - ik(\bar{\hat{\rho}}\hat{u} + \hat{\rho}\bar{\hat{u}})$$
$$= k^2 A(k^2)|\hat{u}|^2 + ik\bar{\hat{u}}(-k^2 B(k^2)\hat{\rho}).$$

But now use the relation $\frac{3}{5}\bar{\hat{\rho}} = ik\bar{c}$ to write the equality as

$$\frac{1}{2}\partial_t\left(\frac{3}{5}|\hat{\rho}|^2 + |\hat{u}|^2 - \frac{3}{5}k^2 B(k^2)|\hat{\rho}|^2\right),$$
$$-ik(\bar{\hat{\rho}}\hat{u} + \hat{\rho}\bar{\hat{u}}) = k^2 A(k^2)|\hat{u}|^2.$$

This is the 'entropy equality in Fourier space. Notice the entropy $\frac{1}{2}\left(\frac{3}{5}|\hat{p}| + |\hat{u}|^2 - \frac{3}{5}k^2 B(k^2)\right)$ and the dissipation $k^2 A(k^2)|\hat{u}|^2$ each have the desired signs (positive and negative, respectively). Since A and B are both negative for $k \neq 0$, integration yields

$$\frac{1}{2}\partial_t \int_{-\infty}^{\infty} \frac{3}{5}|\hat{p}|^2 + |\hat{u}|^2 \, dk + \frac{1}{2}\partial_t \int_{-\infty}^{\infty} -\frac{3}{5}k^2 B(k^2)|\hat{p}|^2 \, dk$$
$$+ \int_{-\infty}^{\infty} \left(\overline{\frac{\partial p}{\partial x}}\right)\hat{u} + \left(\overline{\frac{\partial u}{\partial x}}\right)\hat{p} \, dk$$
$$= \int_{-\infty}^{\infty} k^2 A(k^2)|\hat{u}| \, dk$$

or with an application of Parseval's identity

$$\frac{1}{2}\partial_t \int_{-\infty}^{\infty} \frac{3}{5}|p|^2 + |u|^2 dx + \frac{1}{2}\partial_t \int_{-\infty}^{\infty} -\frac{3}{5}k^2 B(k^2)|\hat{p}|^2 dk$$
$$= \int_{-\infty}^{\infty} k^2 A(k^2)|\hat{u}|^2 dk.$$

The term

$$\int_{-\infty}^{\infty} -\frac{3}{5}k^2 B(k^2)|\hat{p}|^2 dk$$

represents a non-local version of the capillarity, where as the term

$$\int_{-\infty}^{\infty} k^2 A(k^2)|\hat{u}|^2 dk$$

is a non-local version of the viscous dissipation.

• Energy identity

$$\frac{1}{2}\partial_t \int_{-\infty}^{\infty} \frac{3}{\rho}|p|^2 + |u|^2 dx + \frac{1}{2}\partial_t \int_{-\infty}^{\infty} -\frac{3}{\rho}k^2 B(k^2)|\hat{p}|^2 dk$$
$$= \int_{-\infty}^{\infty} k^2 A(k^2)|\hat{u}|^2 dk.$$

Since A, B are negative for $k^2 > 0$ we can interpret the above energy identity as

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

just as given in Korteweg's theory of capillarity. Exact summation of the Chapman–Enskog expansion has yielded a non-local version of Korteweg's theory and not Navier–Stokes theory.

Why is the theory non-local?

Non-locality not because of any physical mechanism but because of the truncatio n of our moment expansion. In fact Boillat and Ruggeri have shown that maximum waves speeds for moment truncation satisfy the inequality

$$V_{max}^2 \geq \frac{6}{5}\sqrt{\frac{5}{3}\frac{k}{m}}\Theta(N - 1/2)$$

where $N =$ number of moments.

Hence, we expect as the number of moments goes to infinity our non-local Korteweg theory would approach a linearization of Korteweg's local theory:

$$\partial_t \rho + \partial_i(\rho u_i) = 0,$$
$$\partial_t(\rho u_i) + \partial_j(\rho u_i u_j) = \partial_j T_{ij},$$

where the Cauchy stress for Korteweg's theory is

$$
\begin{aligned}
T &= T^E + T^V + T^K, \\
T_{ij}^E &= -\rho \psi'(\rho)\delta_{ij}, \quad \rho^2 \psi'(\rho) = p(\rho), \\
T_{ij}^V &= \lambda(\mathrm{tr}D)\delta_{ij} + 2\mu D_{ij} \\
D_{ij} &= \frac{1}{2}\left(\partial_j u_i + \partial_i u_j\right), \\
\lambda &= -\frac{2}{3}\mu, \quad \mu > 0, \\
T_{ij}^K &= \alpha\rho\partial_i(\rho\partial_j\rho) - \alpha\rho\partial_i\rho\partial_j\rho, \quad \alpha > 0.
\end{aligned}
$$

• **The full nonlinear energy balance equation**:

$$\partial_t \left(\frac{1}{2}\rho|u|^2 + \rho\psi(\rho) + \frac{\alpha}{2}\rho\partial_i\rho\partial_i\rho \right) + \partial_j \left[u_j \left(\frac{1}{2}\rho|u|^2 + \rho\psi(\rho) - \frac{\alpha}{2}\rho\partial_i\rho\partial_i\rho \right) \right]$$
$$+ \partial_j[\alpha\rho(\partial_t\rho\partial_j\rho + u_i\partial_i\rho\partial_j\rho)] + \partial_j(u_i T_{ij}) + \mu(\partial_j(u_i\partial_i u_j) - \partial_i(u_i\partial_j u_j))$$
$$= -(\lambda + \mu)(\partial_i u_i)^2 - \mu(\partial_j u_i)(\partial_j u_i)$$
$$\leq 0.$$

(Here repeated indices imply summation.)

Summary

Gorban and Karlin's summation has shown us that we may reasonably conjecture that the sum of Chapman–Enskog expansion will yield a local version of Korteweg's theory of capillarity. Implication of Gorban and Karlin's summation for Hilbert's 6th problem. The whole issue may be seen in the energy balance. If we put the Knudsen number scaling into (reference "3.2") the coefficient α is actually a term $\alpha_0 \varepsilon^2$ and to recover the classical balance of energy of the Euler equation would require the sequence

$$\varepsilon^2 \rho^\varepsilon \partial_i \rho^\varepsilon \partial_i \rho^\varepsilon \to 0$$

in the sense of distributions of $\varepsilon \to 0$

This would require a strong interaction with viscous dissipation. The natural analogy is given by the use of the KdV-Burgers equation:

$$u_t + uu_x = \varepsilon u_{xx} - K\varepsilon^2 u_{xxx}, \qquad (4)$$

where at a more elementary level we see the competition between viscosity and capillarity. The result is known but far from trivial. In the absence of viscosity we have the KdV equation

$$u_t + uu_x = -K\varepsilon^2 u_{xxx}. \qquad (5)$$

and we know from the results of Lax and Levermore that as $\varepsilon \to 0$, solution of (5) will not approach solution of the conservation law

$$u_t + uu_x = 0, \tag{6}$$

after the breakdown time of smooth solutions of (6). On the other hand, addition of viscosity which is sufficiently strong, i.e. K sufficiently small in (4) will allow passage as $\varepsilon \to 0$ to a solution of (6). This has been proven in the paper of M.E. Schonbek.

Are we in the Lax-Levermore case (5) or the Schonbek case (4) with K sufficiently small ? Rewrite hydrodynamics as the second order equation

$$\frac{3}{5}\hat{p}_{tt} + k^2\hat{p} + k^2\left(-A(k^2)\left(\frac{3}{5}\right)\hat{p}_t - k^2 B(k^2)\hat{p}\right) = 0$$

and then attempt to write it in factored form

$$\left(\frac{3}{5}\frac{\partial}{\partial t} + \mu_1(k)\right)\left(\frac{\partial}{\partial t} + \mu_2(k)\right)\hat{p} = -k^2\hat{p}.$$

A comparison yields

$$
\begin{aligned}
\mu_1(k) + \frac{3}{5}\mu_2(k) &= -\frac{3}{5}k^2 A(k^2) \\
\mu_1(k)\mu_2(k) &= -k^4 B(k^2)
\end{aligned}
$$

Define $\hat{v}$ by the formula

$$
\frac{\partial \hat{p}}{\partial t} + \mu_2(k)\hat{p} = ik\hat{v}
$$

system now takes the form

$$
\begin{aligned}
\frac{3}{5}\partial_t \hat{v} &= ik\hat{p} - \mu_1(k)\hat{v} \\
\partial_t \hat{p} &= ik\hat{v} - \mu_2(k)\hat{p}
\end{aligned}
$$

or in physical space-time

$$\frac{3}{5}\partial_t v = -\partial_x p - \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \mu_1(k)\hat{v}(k, t)dk,$$
$$\partial_t p = -\partial_x p - \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \mu_2(k)\hat{p}(k, t)dk.$$

Formulas for $\mu_1(k), \mu_2(k)$ are

$$2\mu_1(k) = -\frac{3}{5}\left(\frac{C}{1-C}\right) \pm \frac{3}{5}i|k|\left(\frac{5C^2 - 16C}{3}\right)^{1/2},$$
$$2\mu_2(k) = -\left(\frac{C}{1-C}\right) \pm i|k|\left(\frac{5C^2 - 16C}{3}\right)^{1/2}.$$

Since $5C^2 - 16C > 0$ (remember $C < 0$), the damping coefficients $\mu_1(k), \mu_2(k)$ are in fact COMPLEX valued reflecting the capillarity effect in the system.

Epilogue

Things are not looking too promising for a possible resolution of Hilbert's 6th problem. It appears in the competition between viscosity and capillarity, capillarity has become a very dogged opponent, and the capillarity energy will not vanish in the limit as $\varepsilon \to 0$. Hilbert's hope may have been justified in 1900, but serious doubts are now apparent. Finally Boltzmann's theory has proven to be a useful model for rarefied gases; Euler's theory has proven to be a useful model for dense gases; maybe they must remain two INDEPENDENT theories and UNIFICATION will NOT succeed for non-smooth (shock) dynamics.

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