Solved and unsolved issues in the theory of shock wave structure

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Physics of gases

Argon  Nitrogen  Carbon dioxide

Translational degree of freedom  Rotational degree of freedom

Monatomic  Diatomic  Polyatomic

Modes of molecular energy.

(r) Vibrational energy $\epsilon_{\text{vib}}$

(f) Electronic energy $\epsilon_{\text{el}}$

1. Kinetic energy
2. Potential energy
(thermal degrees of freedom – 2)

1. Kinetic energy of electrons in orbit
2. Potential energy of electrons in orbit
Shock waves in aerospace

- **Shock waves**: a very thin surface (order of few micro-meter) where the air properties change abruptly, causing the increase of the entropy. Since the speed in the supersonic flow is beyond the speed of sound, air particles cannot obtain the information of what is going on before they actually hit the solid surface. As a result, the kinetic energy of air transforms into the thermal energy, which is always **irreversible** process.
**Shock waves in nature**

- **Interstellar shock waves**: “An understanding of interstellar shock waves is crucial in determining the structure of the interstellar medium. The interstellar medium is a tenuous plasma filling the galactic disk that has a mean density of only about one particle per cubic centimeter” (McKee & Draine, *Science*, 1991).
Physics of shock waves: inner structure

- **Shock waves from 1st law of thermodynamics**
  - Rankine-Hugoniot relation (inviscid upstream and downstream)
    \[ U_t + F_x = 0 \Rightarrow s[U] = [F] \]

- **Inner structure of shock waves from 2nd law of thermodynamics**
Why care about 2nd-order constitutive laws

Conventional 1st-order framework based on Navier-Stokes-Fourier laws

\[ \Pi = -2\eta [\nabla U]^{(2)}, \quad Q = -k \nabla T \]

1st-order constitutive laws are linear and thus remain the same for all flow situations. But they are valid in inner structure of shock waves?

2nd-order framework: major stumbling blocks for theoreticians for a long time

“… is found that the solution breaks down completely, and no solution exists for stronger shocks (specifically, at Mach number \( M=1.65 \))…” (H. Grad 1952)

It was solved by B. C. Eu in 1997 (Phys. Rev. E)

The ultimate origin of the singularity was revealed by R. S. Myong in 2014 (Physics of Fluids)
Derivation of the 2\textsuperscript{nd}-order constitutive laws

(Molecular) Boltzmann kinetic equation: \(10^{23} \quad f(t, \mathbf{r}, \mathbf{v})\)

\[
\left( \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) f(t, \mathbf{r}, \mathbf{v}) = C[f, f_2]
\]

Nonlinear collision integral

Enormous reduction of information

\[
\rho = \langle mf(t, \mathbf{r}, \mathbf{v}) \rangle
\]

\[
\langle \cdots \rangle = \iiint \cdots dv_x dv_y dv_z
\]

\[
\rho \frac{d\mathbf{u}}{dt} + \nabla \cdot (p\mathbf{I} + \Pi) = 0
\]

Conservation laws & constitutive equations: \(13 \quad (\rho, \mathbf{u}, T, \Pi, Q, \cdots)(t, \mathbf{r})\)
Derivation of the 2nd-order constitutive laws

Conservation laws (exact consequence of BTE)

\[
\rho \frac{d}{dt} \begin{bmatrix}
\frac{1}{\rho} \\
u \\
E_t
\end{bmatrix}
+ \nabla \cdot \begin{bmatrix}
-u \\
pI \\
pu
\end{bmatrix}
+ \nabla \cdot \begin{bmatrix}
0 \\
\Pi \\
\Pi \cdot u + Q
\end{bmatrix}
= 0
\]

in conjunction with the (algebraic) 2nd-order constitutive equations

\[
\rho \frac{d(\Pi / \rho)}{dt} + 2[\Pi \cdot \nabla u]^{(2)} + 2p[\nabla u]^{(2)} = -\frac{p}{\mu_{NS}} \Pi q(\kappa_1),
\]

Navier 1st law

\[
\rho \frac{d(Q / \rho)}{dt} + \frac{du}{dt} \cdot \Pi + Q \cdot \nabla u + \Pi \cdot C_p \nabla T + \frac{C_p p \nabla T}{k_{NS}} = -\frac{pC_p}{k_{NS}} Q q(\kappa_1),
\]

Fourier 1st law

\[
q(\kappa_1) = \frac{\sinh \kappa_1}{\kappa_1}, \quad \kappa_1 = T^{1/4} \left( \frac{\Pi : \Pi}{\mu_{NS}} + \frac{Q \cdot Q}{k_{NS}} / T \right)^{1/2}
\]
Topology of 2^{nd}-order constitutive relations

Navier-Fourier

Entropy production parameter

2^{nd}-order laws

Argon

\( \mu_{\text{bulk}} = 0 \)

\( N_2 \)

\( \mu_{\text{bulk}} = \mu_{\text{shear}} \)
2nd-order constitutive relations: Non-Navier laws

Viscous stress /pressure

Grad non-classical model (1952) $F = 1$

Myong non-classical model (1999, 2014)

Navier classical model (1822)

$F = \frac{\sinh(\Pi/p)}{\Pi/p}$

Singularity

Expansion

Compression

Normal (linear viscosity)

Normal (nonlinear viscosity)

$\hat{\Pi} \hat{\Pi}_{NS} + \hat{\Pi}_{NS} = \hat{\Pi}q(\hat{\Pi})$

\[ \frac{\Pi}{p}, \frac{\Pi_{NS}}{p} \]
Physical results: inverse shock thickness

Shock density thickness of argon gas

Shock temperature-density distance

Physical results: shock structure around cylinder

Computed Mach contours over cylinder (Mach 5.48, Kn=0.2)

Unsolved issues

**Diatomic gases:** Difficulty in numerically solving large bulk viscosity case

\[
\begin{align*}
\rho \frac{d}{dt} \begin{bmatrix} 1/\rho \\ u \\ pI \\ E_t \\ pu \end{bmatrix} + \nabla \cdot \begin{bmatrix} -u \\ pI \\ \Pi + \Delta I \\ (\Pi + \Delta I) \cdot u + Q \end{bmatrix} &= \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \Delta : \text{excess normal stress} = -\mu_b \nabla \cdot u
\end{align*}
\]

**Inclusion of vibrational mode:** Need of developing a proper kinetic description of the coupling of rotational and vibrational modes

**Inclusion of radiation**
Unsolved issues

Shock inner structure in magnetohydrodynamics (MHD): Ionized gases in rarefied state under electromagnetic fields

\[
\begin{align*}
\begin{pmatrix}
\rho \\
\rho u \\
B_\perp \\
E
\end{pmatrix}_t + \begin{pmatrix}
\rho u \\
\rho uu + (p + B_\perp \cdot B_\perp / 2)I - B_x B_\perp \\
B_\perp u - B_x v \\
(E + p + B_\perp \cdot B_\perp / 2)u - B_x (B_\perp \cdot v)
\end{pmatrix}
= \begin{pmatrix}
0 \\
D_1 u \\
D_2 B_\perp \\
\Sigma + kT
\end{pmatrix}_x
\end{align*}
\]

where \(2\Sigma = \mu(u \cdot u) + \nu(v \cdot v) + \eta(B_\perp \cdot B_\perp), \quad D_1 = \begin{pmatrix}
\mu & 0 & 0 \\
0 & \nu & 0 \\
0 & 0 & \nu
\end{pmatrix}, \quad D_2 = \begin{pmatrix}
\eta & -\chi \\
\chi & \eta
\end{pmatrix}\)

\(B_\perp\): magnetic field
Unsolved issues

Extension to gas with solid particles (dusty gases)

- Rarefaction wave
- Head
- Tail
- Reflected Shock
- Contact discontinuity
- Boundary particle path
- Reflected compression waves
- Relaxation region
- Shock
- Transmitted Shock
- Red: Pure gas
- Black: Dusty gas