Internal variables and heat conduction in non-equilibrium thermodynamics

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Motivation I.

- Paradox of propagation speed:
  parabolic (infinite) vs. hyperbolic (finite)
- Relativistic models → hyperbolic equations: finite but can be higher than c; parabolic eq.: preserves infinite speed
  In local equilibrium:
  Eckart theory, unstable due to heat conduction
  Out of local equilibrium:Israel-Stewart (hyperbolic?, stability?)
  Müller-Ruggeri (divergence type, hyperbolic), etc...
- Relativistic Fourier equation (parabolic):
  $\gamma(\partial_t - v\partial_x)T - \alpha(\partial_{xx} - 2\frac{v}{c^2}\partial_{xt} + \frac{v^2}{c^4}\partial_{tt})T = 0$
  propagation speed $> c$ is also valid
- In non-relativistic framework:
  Kinetic theory based phenomenology is not perfect
  Non-equilibrium thermodynamics: universal.
  Final benchmark: experiments!

Motivation II.

- Non-classical phenomena
  - Wave propagation ("Second sound") → MCV, GN, GK
  - Ballistic propagation → There is no unified continuum theory! Propagation with speed of sound, mechanical coupling! Kinetic theory is the leading model → phonon hydrodynamics, EIT, RET. Similar to the piston effect from hydrodynamics.
- Obtain compatibility with the kinetic theory → application of internal variables with generalized entropy current
- Heat pulse experiments:
  - NaF samples, on low temperature, test for the modeling capability of non-classical phenomena
  - Inhomogeneous samples, on room temperature, test for the universality.

About kinetic theory - phonon hydrodynamics I.

Interactions $\rightarrow$ distributions

- Normal (N) processes: momentum is conserved
- Resistive (R) processes: momentum is not conserved
- Umklapp-processes: neither the energy, nor the momentum is conserved

Connection to heat conduction

- R-processes are dominant: diffusive propagation (Fourier)
- N-processes are dominant: wave propagation (MCV...)
- Ballistic propagation: heat conduction without interactions!

About kinetic theory - phonon hydrodynamics II.

Momentum series expansion + truncation closure

$$u_{\langle i_1 i_2 \dots i_N \rangle} = \int k n_{\langle i_1 \dots i_n \rangle} f dk.$$

$$\frac{\partial u_{\langle n \rangle}}{\partial t} + \frac{n^2}{4n^2-1} c \frac{\partial u_{\langle n-1 \rangle}}{\partial x} + c \frac{\partial u_{\langle n+1 \rangle}}{\partial x} = \begin{cases} 0 & n = 0 \\ -\frac{1}{\tau_R} u_{\langle 1 \rangle} & n = 1 \\ -\left(\frac{1}{\tau_R} + \frac{1}{\tau_N}\right) u_{\langle n \rangle} & 2 \leq n \leq N \end{cases}$$

It requires at least N=30 momentum equation to obtain the real ballistic propagation speed

Continuum theory - Generalization of heat conduction I

Tensorial internal variable + extended entropy current:

- q^i is a *basic field variable*; Q^{ij} is an *internal variable*
- entropy density: $s(e, q^i, Q^{ij}) = s_e(e) - \frac{m_1}{2} q^i \cdot q^i - \frac{m_2}{2} Q^{ij} \cdot Q^{ij}$
- generalized entropy current: $J^i = b^{ij} q^j + B^{ijk} Q^{jk}$

Entropy production in 1 spatial dimension:

$$\left(b - \frac{1}{T}\right) \partial_x q + (\partial_x b - m_1 \partial_t q)\, q - (\partial_x B - m_2 \partial_t Q)\, Q + B \partial_x Q \geq 0$$

Linear relations between *thermodynamic fluxes* and *forces*, isotropy:

$$\begin{aligned} m_1 \partial_t q - \partial_x b &= -l_1 q, \\ m_2 \partial_t Q - \partial_x B &= -k_1 Q + k_{12} \partial_x q, \\ b - \frac{1}{T} &= -k_{21} Q + k_2 \partial_x q, \\ B &= n \partial_x Q. \end{aligned}$$

Continuum theory - Generalization of heat conduction II

Tensorial internal variable + extended entropy current:

- q^i is a *basic field variable*; Q^{ij} is an *internal variable*
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b - \frac{1}{T} &= -k_{21} Q + \cancel{k_2 \partial_x q}, \\
B &= \cancel{n \partial_x Q}.
\end{aligned}$$

Compatibility with kinetic theory

Properties of the hierarchical structure

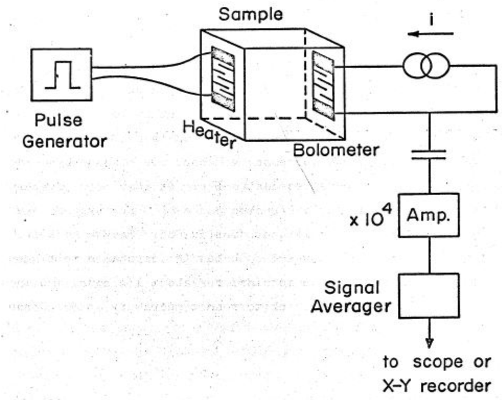
- New quantity: $Q^{ij} \to$ current density of the heat flux
- Effective model in the sense of material parameters
- Incorporates the *ballistic* effect
- Hyperbolic system:
  - finite propagation speeds
  - the existence and uniqueness of the solution

Generalized (dimensionless) equations:

- MCV: $\tau_q \partial_{tt} T + \partial_t T = \partial_{xx} T$
- GK: $\tau_q \partial_{tt} T + \partial_t T = \partial_{xx} T + \kappa^2 \partial_{txx} T$
- Green-Naghdi: $\tau_q \partial_{tt} T = \partial_{xx} T + \kappa^2 \partial_{txx} T$, etc...
- Ballistic-conductive:
  $\tau_q \tau_Q \partial_{ttt} T + (\tau_q + \tau_Q) \partial_{tt} T + \partial_t T = \partial_{xx} T + (\kappa^2 + \tau_Q) \partial_{txx} T$

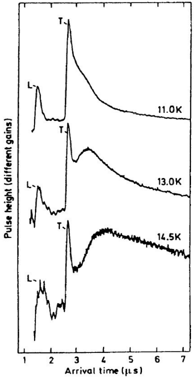
Experiments I.

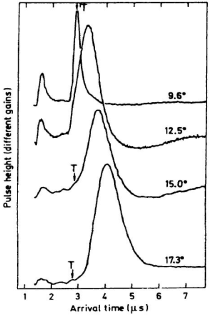
What is the heat pulse experiment?!



Experiments II.

Beyond the phenomenon of second sound $\rightarrow$ ballistic propagation





Jackson - Walker - McNelly experiments on NaF material (1968-70).
The 3 propagation modes can be clearly distinguished!

How can it be modeled?
Kinetic theory + RET: phonon hydrodynamics

Important details

Well-documented series of experiments...but

- The samples can be hardly distinguished (by peak thermal conductivity and sample length) → problematic identification of thermal conductivity → McNelly's PhD thesis makes it clear
- The temperature dependency of material parameters
- Cooling effect during propagation:

$$\partial_t e + \nabla \cdot \mathbf{q} = -\alpha (T - T_0),$$

The ballistic-conductive model I.

System of equations in *dimensionless* form:

$$
\begin{aligned}
\tau_\Delta \frac{\partial T}{\partial t} + \frac{\partial q}{\partial x} &= 0, \\
\tau_q \frac{\partial q}{\partial t} + q + \tau_\Delta \frac{\partial T}{\partial x} + \kappa \frac{\partial Q}{\partial x} &= 0, \\
\tau_Q \frac{\partial Q}{\partial t} + Q + \kappa \frac{\partial q}{\partial x} &= 0.
\end{aligned}
$$

$\kappa \rightarrow$ can be used to adjust the speed of ballistic propagation

Finite difference discretization

- Explicit scheme $\rightarrow$ stability conditions with von Neumann method and Jury criterion.

The ballistic-conductive model II. - IC&BC

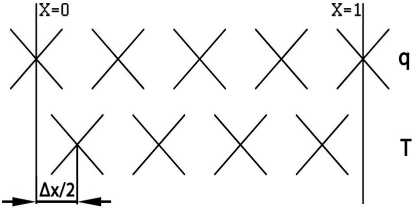
Initial conditions

All fields are zero at t=0.

Boundary conditions

Only for the field of heat flux → *discretization* method!

$$q(t, x=0) = \begin{cases} 1 - cos(2\pi \cdot \frac{t}{t_{pulse}}) & \text{if } 0 < t \leq t_{pulse} \\ 0 & \text{if } t > t_{pulse} \end{cases}$$



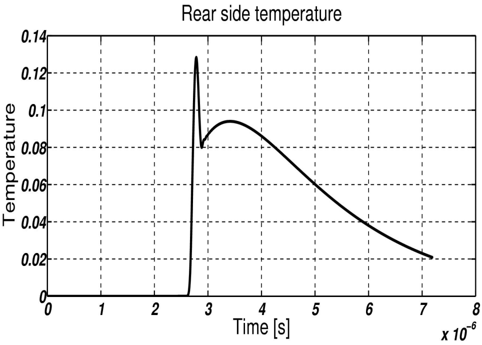
Shifted fields:
One goes from $x = 0$ to $x = 1$, the others shifted by $\frac{\Delta x}{2}$.

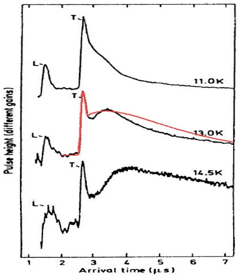
The ballistic-conductive model - Solutions I.

Material parameters:

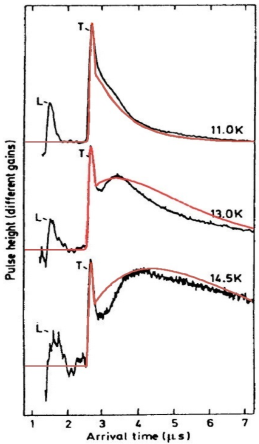
$$k = 10200 \frac{W}{mK}, c = 1.8 \frac{J}{kgK}, \rho = 2866 \frac{kg}{m^3}$$

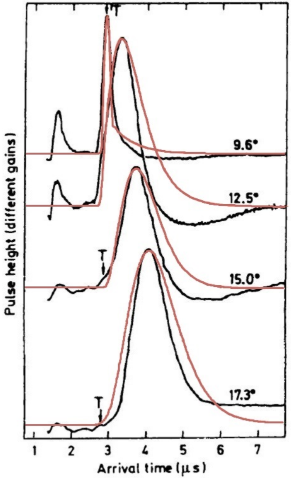
$$\tau_q = 0.355 \mu s, \tau_Q = 0.21 \mu s \text{ and } L = 7.9 mm, \Delta t = 0.24 \mu s$$





The ballistic-conductive model - Solutions II.





"Death match" of different descriptions I.

Phonon hydrodynamics (RET) vs NET+IV

At least N=30 momentum eqs. vs 3 eqs.

No. of fitted parameters: 2 relaxation time vs. 2+1 parameters

Solved on semi-infinite region vs real domain

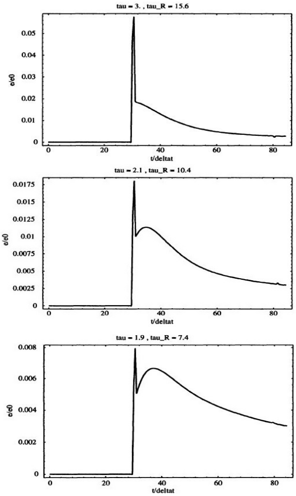
Relative amplitudes: false vs true

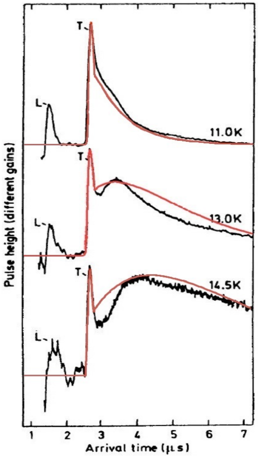
Summary: RET results are more like model testing than fitting;

Wrong: heat pulse length, sample size, thermal conductivity

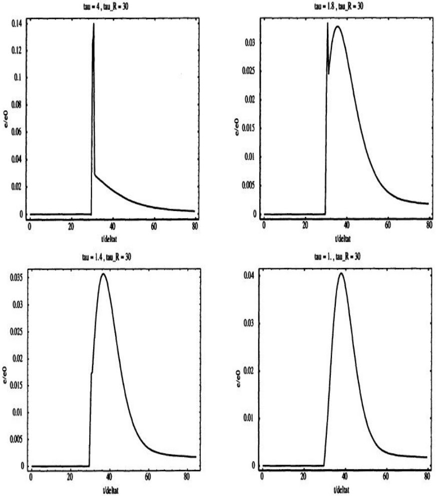
Is the RET model appropriate? Can not be decided.

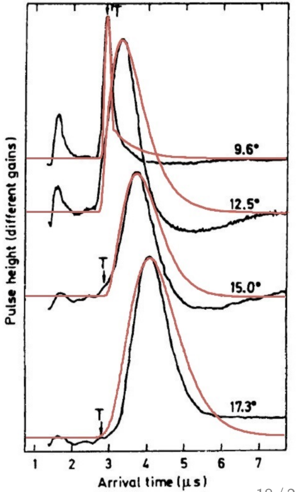
"Death match" of different descriptions II.





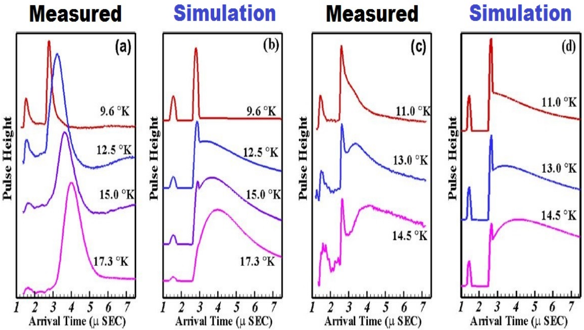
"Death match" of different descriptions III.



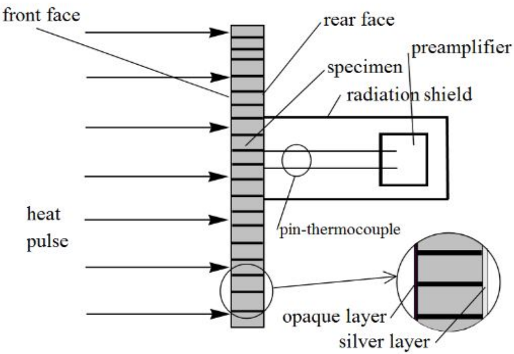


"Death match" of different descriptions IV.

Hybrid phonon gas model of Y. Ma vs NET+IV
Longitudinal signal: artificial extension vs simplified model
Fitted parameters: 2 relaxation time vs 2+1
Boundary conditions: no information vs effective cooling
Wrong thermal conductivity, no information about the others.



What about on room temperature?



Arrangement of the measurement, made at DEE BME

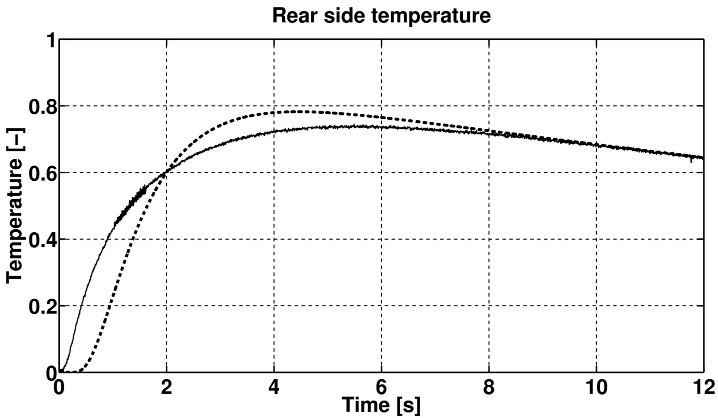
Simplified B-C model ($\tau_Q = 0$): Guyer-Krumhansl equation

$$\cancel{\tau_q \tau_Q \partial_{ttt} T} + (\tau_q + \cancel{\tau_Q})\partial_{tt} T + \partial_t T = \partial_{xx} T + (\kappa^2 + \cancel{\tau_Q})\partial_{txx} T$$

Over-diffusive phenomenon I.

Measurement on room temperature, metal foam sample

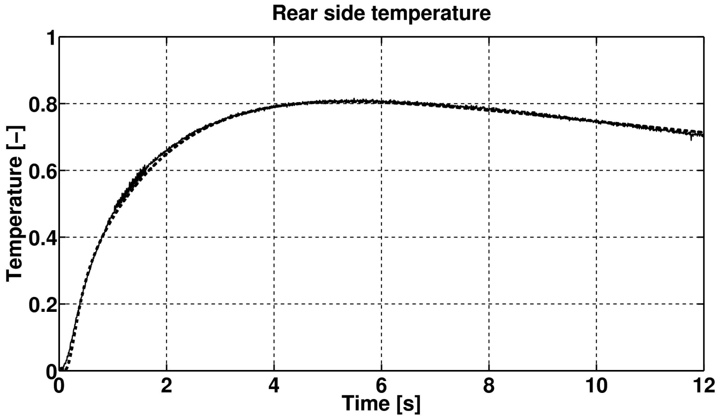
$\tau_q \partial_{tt} T + \partial_t T = \partial_{xx} T + \kappa^2 \partial_{txx} T$, Fourier equation



Over-diffusive phenomenon II.

Measurement on room temperature, metal foam sample

$\tau_q \partial_{tt} T + \partial_t T = \partial_{xx} T + \kappa^2 \partial_{txx} T$, Guyer-Krumhansl equation



Thank you for your kind attention!