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**Vita(, Morte) e Miracoli  
dello Spostamento Termico**

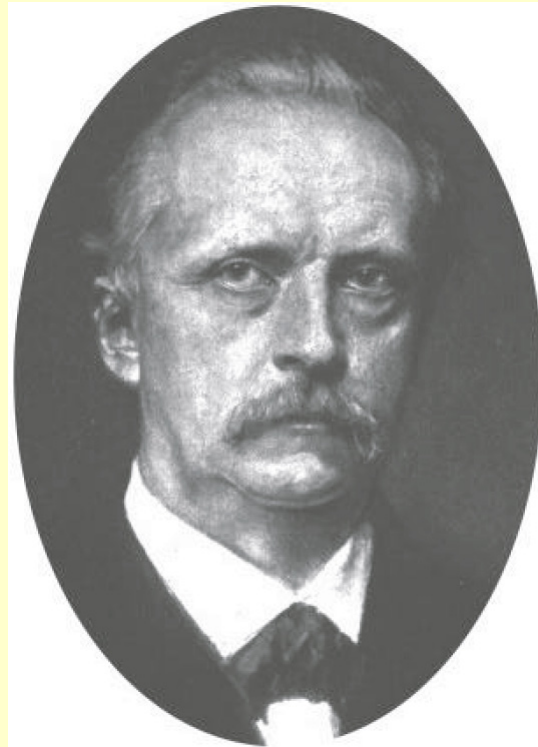
**“A Thermodynamics Day”**

**Padova, 5 giugno 2009**

# VITA

**Thermal displacement, what the hell is that?**

*In principio erat* **HELMHOLTZ** (1821-1894)



- **H von H**, Prinzipien der Statik monocyclischer Systeme (**1884**)
- **H von H**, Studien zur Statik monocyclischer Systeme (**1884**)

## *In fine (?) erat GAM*



- C. Dascalu & GAM, The thermoelastic material-momentum equation. J. Elasticity 39, 201-212 (1995)
- ...

Given that *in principio* erat **Helmholtz** and  
*in fine* erat **GAM**,

Q1. Was there anything *in medio*?

Q2. What comes next?

Before we try and answer, ...

... back to H von H



Ludwig Knaus pinxit

Nr. 1583

Helmholtz

Photographische Gesellschaft in Berlin

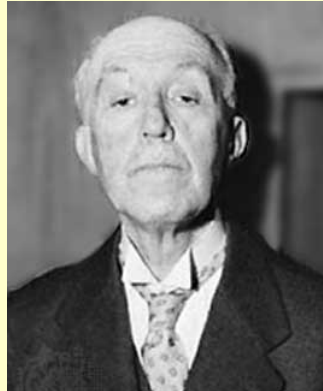
with the help of **Cornelius Lanczos**<sup>\*</sup> and of ...

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<sup>\*</sup> **C. L.**, **The Variational Principles of Mechanics**, Dover, 1986



# Louis de Broglie (1892-1987)



**L de B**, *La Thermodynamique de la particule isolée (ou Thermodynamique cachée des particules)*, Gauthier-Villars, Paris (1964)

# Helmholtz's *Monocyclic* Lagrangian Systems. 1

Consider a lagrangian where the  $n$ -th coordinate is missing:

$$L = L(q_1, \dots, q_{n-1}, \cancel{q_n}; \dot{q}_1, \dots, \dot{q}_n; t).$$

Then,

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_n} \right) = 0 \quad \Leftrightarrow \quad p_n = \frac{\partial L}{\partial \dot{q}_n} = c_n, \text{ a motion constant} \quad \Rightarrow$$

$$\dot{q}_n = f(q_1, \dots, q_{n-1}; \dot{q}_1, \dots, \dot{q}_{n-1}; c_n; t). \quad (*)$$

## Strategy

- With the use of  $(*)$ , obtain  $t \mapsto (q_1(t), \dots, q_{n-1}(t))$ , the time evolution of the ‘**slow**’ coordinates;
- having this information, revert to  $(*)$ , and obtain the time evolution of the ‘**fast**’ coordinate  $q_n$  by quadrature.

Note    A fast coordinate is not observable, its time rate is.

## Helmholtz's *Monocyclic* Lagrangian Systems. 2

Require the **action**  $\mathcal{A} = \int_{t_1}^{t_2} L(q_1, \dots, q_{n-1}; \dot{q}_1, \dots, \dot{q}_n; t) dt$  **be stationary under the constraint**

$$\dot{q}_n = f(q_1, \dots, q_{n-1}; \dot{q}_1, \dots, \dot{q}_{n-1}; c_n; t). \quad (*)$$

**Formally,**

$$\delta \left( \int_{t_1}^{t_2} (L(q_1, \dots, q_{n-1}; \dot{q}_1, \dots, \dot{q}_n; t) + \lambda \dot{q}_n) dt \right) = 0$$

**implies**

$$\lambda = -\frac{\partial L}{\partial \dot{q}_n} = -p_n = -c_n.$$

**Accordingly, one can introduce the *modified lagrangian***

$$\overline{L}(q_1, \dots, q_{n-1}; \dot{q}_1, \dots, \dot{q}_{n-1}; c_n; t) =: L(q_1, \dots, q_{n-1}; \dot{q}_1, \dots, \dot{q}_n; t) - c_n \dot{q}_n,$$

**where (\*) specifies  $\dot{q}_n$ .**

# Helmholtz's *Monocyclic* Lagrangian Systems. 3

Split  $L = K - U$ , with  $U = U(q_1, q_2, \dots, q_{n-1}; t)$  the *potential energy* and

$$K = \frac{1}{2} \sum_{i=1}^{n-1} a_{ik} \dot{q}_i \dot{q}_k + \left( \sum_{i=1}^{n-1} a_{in} \dot{q}_i \right) \dot{q}_n + \frac{1}{2} a_{nn} \dot{q}_n^2$$

the *kinetic energy*. This implies that  $\bar{L} = \bar{K} - \bar{U}$ , with

$$\bar{K} := \frac{1}{2} \sum_{i=1}^{n-1} a_{ik} \dot{q}_i \dot{q}_k + \frac{1}{2} \left( \sum_{i=1}^{n-1} a_{in} \dot{q}_i \right)^2 + a_{nn}^{-1} c_n \sum_{i=1}^{n-1} a_{in} \dot{q}_i, \quad \bar{U} := U + \frac{1}{2} a_{nn}^{-1} c_n^2.$$

- If  $a_{in} \neq 0$ , then (i) *kinetic coupling* between fast variable  $q_n$  and slow variable  $q_i$ ; (ii) *gyroscopic term*  $a_{in} \dot{q}_i$  in the kinetic energy.
- *potential energy augmented by a positive contribution of kinetic origin*, a manifestation of the ‘ghost’ variable  $q_n$ , the only manifestation in case of no kinetic coupling.

# Helmholtz's Heat Theorem. 1

Stripped-to-the-bones motion equations are:

$$\frac{\partial L}{\partial q_s} + \cancel{\mathbb{Y}_s} = 0, \quad -\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_f} \right) + g_f = 0 \Leftrightarrow -\dot{p}_f + g_f = 0$$

(one fast coordinate, one slow;  $g_f \equiv$  only external force).

The incremental working performed on the system is:

$$dQ = g_f dq_f = \dot{p}_f \dot{q}_f dt = \dot{q}_f dp_f \Rightarrow \frac{dQ}{2K} = d(\log p_f).$$

Formally, on setting

$$2K =: \text{temperature } T \quad \text{and} \quad \log p_f := \text{entropy } S,$$

we have:

$$\frac{dQ}{T} = dS,$$

with '*coldness*'  $T^{-1}$  as the integrating factor. Note that this conclusion does not depend on the form of the potential energy.

# Helmholtz's Heat Theorem. 2

When generalized so as to apply to a *multidimensional ergodic system*, this result takes the form of the *heat theorem*:

$$\frac{dE + PdV}{T} = dS_{\Phi}, \quad (1)$$

where  $S_{\Phi}$  is the *volume entropy*:

$$S_{\Phi}(E) := \log \Phi(E), \quad \Phi(E) := \int_{P_h S_p} H(E - \mathcal{H}(\mathbb{Q}, \mathbb{P})) d\mathbb{Q}d\mathbb{P},$$

$$\text{and} \quad T := 2 \langle K \rangle, \quad E = K + U, \quad P := \left\langle -\frac{\partial U}{\partial q} \right\rangle.$$

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**Recall that**

$$\Phi'(E) = \Omega(E) = \int_{P_h S_p} \delta(E - \mathcal{H}(\mathbb{Q}, \mathbb{P})) d\mathbb{Q}d\mathbb{P},$$

$$\langle F \rangle(E) := \frac{1}{\Omega(E)} \int_{P_h S_p} F(\mathbb{Q}, \mathbb{P}) \delta(E - \mathcal{H}(\mathbb{Q}, \mathbb{P})) d\mathbb{Q}d\mathbb{P}.$$

N° 17

# La Thermodynamique de la particule isolée

(ou Thermodynamique cachée des particules)

par Louis de BROGLIE  
de l'Académie française,  
Secrétaire perpétuel de l'Académie des Sciences



gv

[from p. 63] “Le schéma canonique de la Thermodynamique de Helmholtz part essentiellement de l'introduction d'une variable  $\alpha$  dont la température est la dérivée par rapport au temps, mais la signification de la variable  $\alpha$  reste mystérieuse.”

**Thermal displacement, additional references**  
**(just to hint at what erat *in medio*)**



# References from the physical literature

- **M. von Laue**, *Relativitätstheorie*, Vol. 1, Braunschweig (1921).
- **D. van Dantzig**, On the phenomenological thermodynamics of moving matter. *Physica* 6, 673-704 (1939).
- ...
- **V.E. Kuzmichev** and **V.V. Kuzmichev**, Accelerating Quantum Universe. *Acta Phys. Pol. B* 39 (2008)

NOTE! For von L., **thermacy** = *minus* **thermal displacement**; van D. calls the thermal displ. **thermasy**, just as the authors to follow, who are in search of a **hamiltonian structure for relativistic perfect fluids**:

- **D. Bao**, **J. Marsden**, and **R. Walton**, The Hamiltonian Structure of General Relativistic Perfect Fluids. *Comm. Math. Phys.* (1985)
- **J. Kijowski**, **A. Smólski**, and **A. Górnicka**, Hamiltonian theory of self-gravitating perfect fluid ... *Phys. Rev. D* 41 (1990)
- ...

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- **G.A. Maugin**, Towards an analytical mechanics of dissipative materials. *Rend. Sem. Mat. Univ. Pol. Torino* 58 (2), 171-180 (2000).
- **G.A. Maugin** and **V.K. Kalpakides**, The slow march towards an analytical mechanics of dissipative materials. *Tech. Mech.* 22 (2), 98-103 (2002).
- **G.A. Maugin** and **V.K. Kalpakides**, A Hamiltonian formulation for elasticity and thermoelasticity. *J. Phys. A: Math. Gen.* 35, 10775-10788 (2002).

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- **A.E. Green** and **P.M. Naghdi**, A re-examination of the basic postulates of thermomechanics. Proc. Royal Soc. London A432, 171-194 (1991).
- **A.E. Green** and **P.M. Naghdi**, A demonstration of consistency of an entropy balance with balance of energy.  
ZAMP 42, 159-168 (1991).
- **A.E. Green** and **P.M. Naghdi**, Thermoelasticity without energy dissipation. J. Elasticity 31, 189-208 (1993).
- **V.K. Kalpakides** and **C. Dascalu**, On the configurational force balance in thermomechanics. Proc. R. Soc. London. A458, 3023-3039 (2002).
- **S. Bargmann** and **P. Steinmann**, Theoretical and computational aspects of non-classical thermoelasticity. Comp. Meth. Appl. Mech. Eng. 196, 516-527 (2006).

**MIRACOLI**

# A Virtual-Working Format for Thermomechanics\*

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\* **P. P-G**, Continuum Mechanics and Thermodynamics, Volume 20 (8), pp. 479-487 (2009)

building upon an idea sketched in

**P. P-G** and **A. Tiero**, Un formato tipo lavori virtuali per la termodinamica dei processi omogenei. Proc. XIV Congr. Naz. Meccanica Teor. Appl. (Como, Italy - October 1999)

# The Standard Mechanical & Thermal Structures

- *mechanical* body structure based on

- **Virtual Working Principle**

$$\int_{\mathcal{P}} \mathbf{S} \cdot \nabla \mathbf{v} = \int_{\mathcal{P}} \mathbf{d} \cdot \mathbf{v} + \int_{\partial \mathcal{P}} \mathbf{c} \cdot \mathbf{v}, \quad \mathbf{v} \in \mathcal{V}, \quad \mathcal{P} \subset \mathcal{B},$$

implying **force balance**;

- *thermal* body structure based on

- **energy balance**

$$\dot{\varepsilon} = -\mathbf{div} \mathbf{q} + r,$$

- **entropy imbalance**

$$\dot{\eta} \geq -\mathbf{div} \mathbf{h} + s, \quad \text{with } \mathbf{h} = \vartheta^{-1} \mathbf{q}, \quad s = \vartheta^{-1} r.$$

# Body as a Composition of Mechanical & Thermal Structures. i. Kinetics

- kinetic variables are

- **mechanical displacement**  $u$ , with

$$v = \dot{u} \equiv \text{velocity},$$

- **thermal displacement**  $\alpha$ , with

$$\vartheta = \dot{\alpha} \equiv \text{temperature},$$

defined over *space-time cylinder*  $\mathcal{B} \times (0, T)$

- **process**  $(x, t) \mapsto (u(x, t), \alpha(x, t))$ , with  
 $(v(x, t), \vartheta(x, t)) \equiv \text{realizable velocity pair}$
- $(\delta u(x, t), \delta \alpha(x, t)) \equiv \text{virtual velocity pair}$

# Body as a Composition of Mechanical & Thermal Structures. ii. Dynamics

For  $\mathcal{P}$  a *subbody* of  $\mathcal{B}$ , and  $I = (t_i, t_f)$  a *subinterval* of  $(0, T)$ , dynamics specified by

(i) *internal virtual working*

$$\delta \mathcal{W}^{(i)} = \int_{\mathcal{P} \times I} (\mathbf{s} \cdot \delta \mathbf{u} + \mathbf{S} \cdot \nabla \delta \mathbf{u} + h \delta \alpha + \mathbf{h} \cdot \nabla \delta \alpha),$$

where

- $\mathbf{s}$  and  $\mathbf{S} \equiv$  0-th and 1-st order mechanical interactions
- $h$  and  $\mathbf{h} \equiv$  0-th and 1-st order thermal interactions



## Note

Treatments of mechanical and thermal entities should be kept *as parallel as possible*. *Parallelism broken by*

- *invariance requirements*

in a *galilean observer change*,

$$v \mapsto v^+ = v + t, \quad \dot{\alpha} \mapsto \dot{\alpha}^+ = \dot{\alpha}.$$

Thus, translational invariance of  $\delta\mathcal{W}^{(i)}$  implies a symmetry-breaking conclusion:

*the 0th order stress  $s$  is null.*

- *habit*

*habitual entropy flux = minus the 1-st order thermal interaction  $h$ .*

(ii) *external virtual working*

$$\begin{aligned}\delta\mathcal{W}^{(e)} = & \int_{\mathcal{P} \times I} (\mathbf{d} \cdot \delta\mathbf{u} + \mathbf{p} \cdot \overline{\dot{\delta\mathbf{u}}} + s \delta\alpha + \eta \overline{\dot{\delta\alpha}}) \\ & + \int_{\partial\mathcal{P} \times I} (\mathbf{c} \cdot \delta\mathbf{u} + c \delta\alpha) + \int_{\mathcal{P} \times \partial I} [\![\mathbf{p} \cdot \delta\mathbf{u} + \eta \delta\alpha]\!]\end{aligned}$$

- $(\mathbf{d}, \mathbf{c})$  &  $(s, c) \equiv$  *mech.* & *therm.* (distance, contact) interactions;
- $\mathbf{p} \equiv$  **momentum**,  $(S\mathbf{n} \equiv$  **momentum flux**)  
 $\mathbf{d} \equiv$  **momentum source**  $\equiv$  (noninertial distance force);
- $\eta \equiv$  **entropy**,  $(h \cdot \mathbf{n} \equiv$  **entropy flux**)  $s \equiv$  **entropy source**;
- $\mathbf{c} \equiv$  **contact force**,  $c \equiv$  **contact heating**;
- $\mathbf{p}_f, \dots, \eta_i \equiv$  **mechanical** & **thermal** *external actions*, at time boundaries of  $\mathcal{P} \times I$ :

$$\begin{aligned}\int_{\partial I} [\![\mathbf{p} \cdot \delta\mathbf{u} + \eta \delta\alpha]\!] := & \mathbf{p}_f(x) \cdot \delta\mathbf{u}(x, t_f) + \eta_f(x) \delta\alpha(x, t_f) \\ & + \mathbf{p}_i(x) \cdot \delta\mathbf{u}(x, t_i) + \eta_i(x) \delta\alpha(x, t_i) .\end{aligned}$$

# Notes

- Just as  $\alpha$  called *thermal displacement* to allude to role analogy with mechanical displacement  $u$ ,  
why not to regard  $\eta$  as the *thermal momentum*, by analogy with the mechanical momentum  $p$ ?
- Just as  $p$  thought of as measuring *reluctance to quiet*,  
why not to think of  $\eta$  as measuring *reluctance to order*?

# The Virtual Working Axiom

**(VW)** The internal and the external working should be equal:

$$\delta\mathcal{W}^{(i)} = \delta\mathcal{W}^{(e)},$$

*for each virtual velocity pair defined over the closure of any subcylinder  $\mathcal{P} \times I$  of  $\mathcal{B} \times (0, T)$  and such as to vanish at the end of  $I$  itself.*

# Implications of VW Axiom

- *momentum* and *entropy balances*:

$$\dot{p} = \text{Div } S - s + d, \quad \dot{\eta} = \text{Div } h - h + s \quad \text{in } \mathcal{P} \times I$$

- *initial conditions*:

$$p(x, t_i) = p_i(x), \quad \eta(x, t_i) = \eta_i(x) \quad \text{for } x \in \mathcal{P}$$

- *boundary conditions* on  $\partial\mathcal{P} \times I$ :

$$Sn = c \quad \equiv \quad \text{balance of contact forces: } c + S(-n) = 0;$$

$$h \cdot n = c \quad \equiv \quad \text{continuity cond. on contact heating: } c = (-h) \cdot (-n)$$

establishing  $-h$  as a measure of specific *entropy influx* at a point of an oriented surface of normal  $n$ .

# Conservation of Internal Action. Preliminaries

An integral consequence of momentum and entropy balances is:

$$W(\mathcal{P}) + H(\mathcal{P}) = \frac{d}{dt} \left( \int_{\mathcal{P}} (\mathbf{p} \cdot \mathbf{v} + \eta \vartheta) \right) + \int_{\mathcal{P}} \textcolor{red}{stuff},$$

where

- *noninertial working*  $W(\mathcal{P}) := \int_{\mathcal{P}} \mathbf{d} \cdot \mathbf{v} + \int_{\partial \mathcal{P}} \mathbf{c} \cdot \mathbf{v},$

- *heating*  $H(\mathcal{P}) := \int_{\mathcal{P}} s \vartheta + \int_{\partial \mathcal{P}} c \vartheta,$

- 

$$\int_{\mathcal{P}} \textcolor{red}{stuff} = \frac{d}{dt} \Phi(\mathcal{P}), \text{ where } \textcolor{red}{internal action} \quad \Phi(\mathcal{P}) := \int_{\mathcal{P}} \varphi,$$

whence

$$\textcolor{red}{stuff} = \mathbf{s} \cdot \mathbf{v} + \mathbf{S} \cdot \nabla \mathbf{v} - \mathbf{p} \cdot \dot{\mathbf{v}} + h \vartheta + \mathbf{h} \cdot \nabla \vartheta - \eta \dot{\vartheta} := \dot{\varphi}.$$

# The Axiom of Conservation of Internal Action

**(CIA)** *In a cycle, the noninertial working plus the heating supplied to or extracted from  $\mathcal{P}$  sum to null:*

$$\oint (W(\mathcal{P}) + H(\mathcal{P})) = 0 .$$

Equivalently,

**(CIA)'** *In a cycle, the internal action is conserved:*

$$\oint \Phi(\mathcal{P}) = 0 .$$

# Implications of CIA Axiom. The 1st Law

For  $\tau \equiv$  specific *total energy*:

$$\tau := \varphi + \mathbf{p} \cdot \mathbf{v} + \eta \vartheta, \quad T(\mathcal{P}) := \int_{\mathcal{P}} \tau,$$

we have:

$$\dot{T}(\mathcal{P}) = W(\mathcal{P}) + H(\mathcal{P}), \quad \text{the } \underline{\text{First Law}} \text{ of TD.}$$



To see this,

- set *entropy inflow*  $(-h, s)$  proportional to *energy inflow*  $(-q, r)$  through *coldness*:

$$h = \vartheta^{-1} q, \quad s = \vartheta^{-1} r;$$

- accept standard notion of specific *kinetic energy*  $\kappa$ :

$$\kappa := \frac{1}{2} p \cdot v, \quad \text{with } \dot{p} \cdot v = p \cdot \dot{v}, \quad (\text{so that } \dot{\kappa} + (-\dot{p}) \cdot v = 0).$$

- set

$$\varepsilon := \tau - \kappa, \quad \varphi := \psi - \kappa,$$

and interpret

- $\varepsilon \equiv$  specific *internal energy*
- $\psi \equiv$  specific *Helmholtz free energy*  $= \varepsilon - \eta \vartheta$ ,

whence the interpretations for both the *total energy*  $\tau$  and the *internal action*  $\varphi$ .

# The Dissipation Axiom

**(D)** *Whatever the process*  $(x, t) \mapsto (\mathbf{u}(x, t), \alpha(x, t))$ ,

$$h \dot{\alpha} \leq 0$$

*over the space-time cylinder*  $\mathcal{B} \times (0, T)$ .

# Implications of D Axiom. The 2nd Law

- Main implication is the generalized *dissipation inequality*:

$$\dot{\psi} \leq -\eta \dot{\vartheta} + \mathbf{h} \cdot \nabla \vartheta + \mathbf{s} \cdot \mathbf{v} + \mathbf{S} \cdot \nabla \mathbf{v} .$$

- **If**  $\vartheta \geq 0$  (an unnecessary assumption so far),  
**then** *entropy balance & D axiom imply*:

$$\dot{\eta} \geq \operatorname{div} \mathbf{h} + s \quad (\textit{entropy imbalance} \equiv \text{the } \underline{\text{Second Law}} \text{ of TD}) .$$

- *Standard dissipation inequality & entropy imbalance follow for*

$$\mathbf{h} = -\vartheta^{-1} \mathbf{q} , \quad s = \vartheta^{-1} r ; \quad \mathbf{s} = \mathbf{0} .$$

**Thermal displacement, what the hell is that?**

**Is there a statistical notion of thermal displacement?**

## Listening to Green & Naghdi (1991):

“The **temperature**  $T$  (on the macroscopic scale) is generally regarded as representing (on the molecular scale) some ‘mean’ velocity magnitude or ‘mean’ (kinetic energy)<sup>1/2</sup>. With this in mind, we introduce a scalar  $\alpha = \alpha(X, \tau)$  through an integral of the form

$$\alpha = \int_{t_0}^t T(X, \tau) d\tau + \alpha_0, \quad (7.3)$$

where  $t_0$  denotes some reference time and the constant  $\alpha_0$  is the initial value of  $\alpha$  at time  $t_0$ . In view of the above interpretation associated with  $T$  and the physical dimension of the quantity defined by (7.3), the variable  $\alpha$  may justifiably be called thermal displacement magnitude or simply **thermal displacement**. Alternatively, *we may regard the scalar  $\alpha$  (on the macroscopic scale) as representing a ‘mean’ displacement magnitude on the molecular scale* [italics are mine] and then  $T = \dot{\alpha}$ .”

## Listening to Kalpakides & Dascalu (2002):

“Taking the view of Green & Naghdi, we consider that  $\alpha(X, t)$  *represents a second motion of the continuum, taking place at a different scale from the macroscopic motion  $y(X, t)$* . This could be *a continuous representation of the lattice vibration*, a phenomenon of quantum-mechanical origin. [my italics] *This justifies us to postulate complete independence in the corresponding observers of the two motions, hence to introduce two kind[s] of observer changes ...*”

# Summing up:

- (Green & Naghdi)

- primary variable: either temperature or thermal displacement;
- both variables should be given a statistical interpretation as some ensemble average.

- (Kalpakides & Dascalu)

- thermal displacement as primary variable;
- reference to lattice vibration appropriate only when thinking of a lattice is;
- use of *microscopic observer changes*:

$$v \mapsto v^+ = v, \quad \dot{\alpha} \mapsto \dot{\alpha}^+ = \dot{\alpha} + \beta, \quad \beta = \text{an arbitrary scalar},$$

has equivalent consequences to my use of virtual velocities  $\delta\alpha$ .  
(Recall: *galilean o. c.*,  $v \mapsto v^+ = v + t$ ,  $\dot{\alpha} \mapsto \dot{\alpha}^+ = \dot{\alpha}$ .)