Weakly nonlocal non-equilibrium thermodynamics

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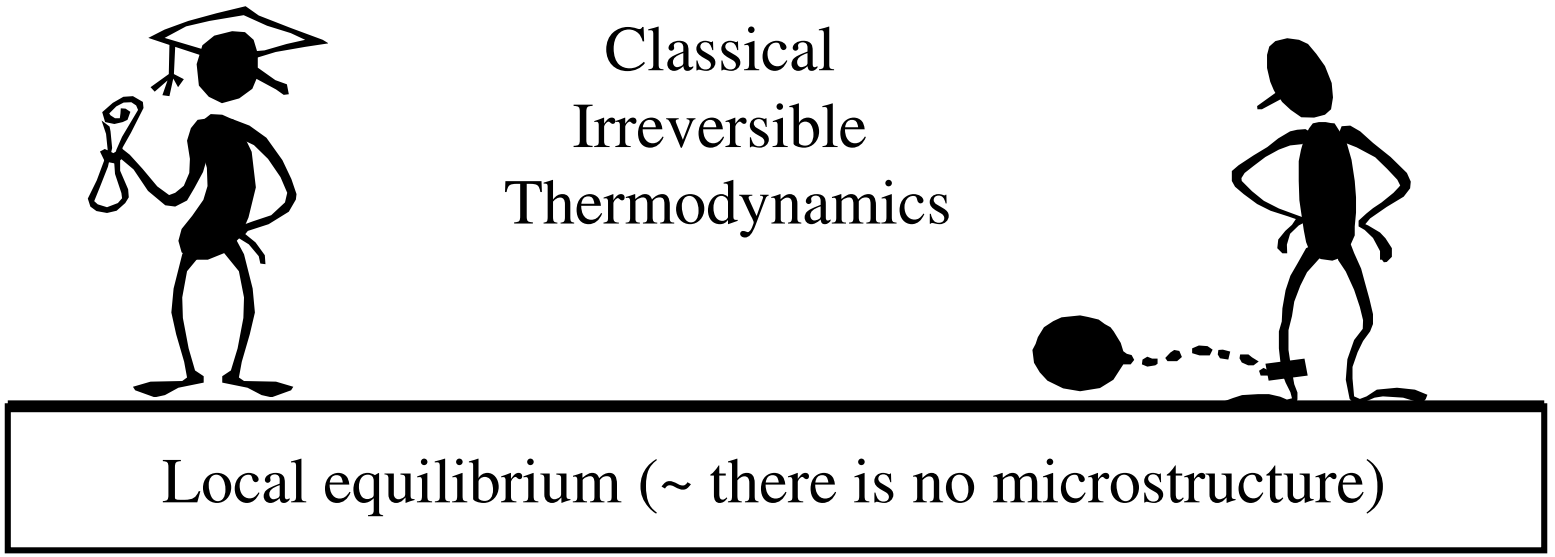
- Non-equilibrium thermodynamics
  - Beyond local equilibrium and local state
  - Exploitations of the Second Law - Liu procedure
- Examples
  - Guyer-Krumhansl equation
  - Ginzburg-Landau equation
  - One component fluid mechanics - quantum (?) fluids
- Conclusions



Beyond local equilibrium (nonlocality):

- in time (memory effects) → dynamic variables
- in space (structure effects) → ?

Method: local state and beyond …

Nonlocalities:

	Space	Time
Strongly nonlocal	Space integrals	Memory functionals
Weakly nonlocal	*Gradient dependent constitutive functions*	Rate dependent constitutive functions
Relocalized	*Current multipliers*	Internal variables

Restrictions from the Second Law.

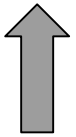
Non-equilibrium thermodynamics

$$\dot{\mathbf{a}} + \nabla \cdot \mathbf{j}_a = \sigma_a$$ basic balances (and more) $$\mathbf{a} = (\rho, \rho\mathbf{v}, \ldots)$$

– basic state: $\mathbf{a}$

– constitutive state: $C = (\mathbf{a}, \dot{\mathbf{a}}, \nabla\mathbf{a}, \ldots)$

– constitutive functions: $\mathbf{j}_a(C)$

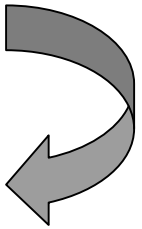


weakly nonlocal

<u>Second law:</u>

$$\dot{s}(C) + \nabla \cdot \mathbf{j}_s(C) = \sigma_s \geq 0$$

Constitutive theory



(universality)

Method: Liu procedure

Speciality: constructive

Weakly nonlocal extended thermodynamics

$$\partial_t u + \nabla \cdot \mathbf{q} = 0$$
$$\partial_t \mathbf{q} + G = 0$$
$$\partial_t s + \nabla \cdot \mathbf{j}_s \geq 0$$

$(u, \nabla u, \mathbf{q}, \nabla \mathbf{q}, \nabla^2 \mathbf{q})$ state space

$(G, s, \mathbf{j}_s)$ constitutive functions

local state: $s(u, \mathbf{q})$

Liu procedure (Farkas's lemma):

$$\mathbf{j}_s(u, \mathbf{q}, \nabla \mathbf{q})$$

$$\sigma_s = \nabla \cdot \mathbf{j}_s - \partial_u s \nabla \cdot \mathbf{q} - \partial_{\mathbf{q}} s G \geq 0$$

solution?

$$s(u,\mathbf{q}) = s_0(u) - \frac{1}{2}\mathbf{q}\cdot\mathbf{m}(u,\mathbf{q})\cdot\mathbf{q}$$ extended (Gyarmati) entropy

$$\mathbf{j}_s(u,\mathbf{q},\nabla\mathbf{q}) = \mathbf{B}(u,\mathbf{q},\nabla\mathbf{q})\cdot\mathbf{q}$$ entropy current (Nyíri)

(**B** – *current multiplier*)

$$\sigma_s = (\mathbf{B} - \partial_u s\mathbf{I}) : \nabla\mathbf{q} + (\nabla\cdot\mathbf{B} + G\cdot\hat{\mathbf{m}})\cdot\mathbf{q} \geq 0$$

$$\mathbf{B} - \partial_u s\mathbf{I} = L_{11}\nabla\mathbf{q} + L_{12}\mathbf{q}$$

$$\nabla\cdot\mathbf{B} + G\cdot\hat{\mathbf{m}} = L_{21}\nabla\mathbf{q} + L_{22}\mathbf{q}$$

$$\hat{\mathbf{m}}\cdot\partial_t\mathbf{q} + \nabla\cdot(L_{11}\nabla\mathbf{q} + L_{12}\mathbf{q} + \partial_1 s\mathbf{I}) = L_{21}\nabla\mathbf{q} + L_{22}\mathbf{q}$$

balance?

local?

Weakly nonlocal internal variables

Ginzburg-Landau (variational):

$$F(\xi)=\int\left(f(\xi)+\frac{\lambda}{2}(\nabla\xi)^2\right)dV \quad \Rightarrow \quad \delta_\xi F = f'(\xi)-\lambda\Delta\xi$$

$$\dot{\xi}=-l\,\delta_\xi F$$

$$\dot{\xi}=-l\left(f'(\xi)-\lambda\Delta\xi\right)$$

– Second Law
– Variational (!)
– $+\,k\Delta\dot{\xi}$

Ginzburg-Landau (thermodynamic, relocalized)

$$\partial_t \xi + F = 0$$
$$\partial_t s + \nabla \cdot \mathbf{j}_s \geq 0$$

$(\xi, \nabla\xi, \nabla^2\xi)$ state space

$(F, s, \mathbf{j_s})$ constitutive functions

local state $s(\xi)$

Liu procedure (Farkas's lemma)

$$\mathbf{j}_s(\xi, \nabla\xi)$$

$$\sigma_s = \nabla \cdot \mathbf{j}_s - s' F \geq 0$$

?

$$\mathbf{j}_s(\xi, \nabla\xi) = \mathbf{B}(\xi, \nabla\xi)\partial_\xi s$$ current multiplier

$$\sigma_s = \mathbf{B}\cdot\nabla s' + (\nabla\cdot\mathbf{B} - F)s' \geq 0$$

$$\mathbf{B} = L_{11}s' + L_{12}\nabla s'$$

$$\nabla\cdot\mathbf{B} - F = L_{21}\nabla s' + L_{22}s'$$

isotropy

$$\partial_t\xi = L_{11}\partial_\xi s - \nabla\cdot(L_{22}\nabla\partial_\xi s)$$

$$\dot{\xi} = -l(f'(\xi) - \lambda\Delta\xi)$$

Ginzburg-Landau (thermodynamic, non relocalizable)

$$\partial_t \xi + F = 0$$

$$\partial_t \nabla \xi + \nabla F = 0$$

$$\partial_t s + \nabla \cdot \mathbf{j}_s \geq 0$$

$(\xi, \nabla\xi, \nabla^2\xi)$ state space

$(F, s, \mathbf{j_s})$ constitutive functions

Liu procedure (Farkas's lemma)

$s(\xi, \nabla\xi)$ $\qquad$ $j_s(.) = j_0(\xi, \nabla\xi) - \partial_\xi s \, F(.)$

$$\sigma_s = -(\partial_\xi s - \nabla \cdot \partial_{\nabla\xi} s) F \geq 0$$

$$\partial_t \xi = -L(\partial_\xi s - \nabla \cdot \partial_{\nabla\xi} s)$$

One component weakly nonlocal fluids and quantum mechanics

Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\Delta\psi+V(x)\psi$$

Madelung transformation: $\psi = R\,e^{iS}$

$$\dot{\rho}+\nabla\cdot\mathbf{v}=0$$

$$\rho := R^2 \qquad \mathbf{v} := \frac{\hbar}{m}\nabla S$$

de Broglie-Bohm form:

$$\dot{\mathbf{v}}=-\nabla(U_{QM}+V)$$

$$U_{QM}=-\frac{\hbar^2}{2m^2}\frac{\Delta R}{R}$$

Hydrodynamic form:

$$\rho\dot{\mathbf{v}}+\nabla\cdot\mathbf{P}_{QM}=-\rho\nabla V$$

One component weakly nonlocal fluid

$$\dot{\rho} + \rho \nabla \cdot \mathbf{v} = 0$$
$$\rho \dot{\mathbf{v}} + \nabla \cdot \mathbf{P}(C) = \mathbf{0}$$
$$\rho \dot{s}(C) + \nabla \cdot \mathbf{j}_s(C) \geq 0$$

$(\rho, \mathbf{v})$ basic state

$C_{wnl} = (\rho, \nabla\rho, \nabla\nabla\rho, \mathbf{v}, \nabla\mathbf{v})$

constitutive state

$s(C), \mathbf{j}_s(C), \mathbf{P}(C)$

⇧

constitutive functions

Liu procedure (Farkas's lemma):

$$s(\rho, \mathbf{v}, \nabla\rho) = s_e(\rho, \nabla\rho) - \frac{\mathbf{v}^2}{2} \qquad \mathbf{j}_s = -\mathbf{v} \cdot \mathbf{P} + \ldots$$

$\mathbf{P}^r$ reversible pressure

$$\sigma_s = -\left(\mathbf{P} - \rho^2 \left[\quad - \partial_\rho s \right] \mathbf{I} \quad \right) : \nabla \mathbf{v} \geq 0$$

$$\mathbf{P}^v = \mathbf{P} - \mathbf{P}^r$$

Schrödinger-Madelung fluid

(Fisher entropy)

$$s_{SchM}(\rho, \mathbf{v}, \nabla\rho) = -\frac{\nu_{SchM}}{2}\left(\frac{\nabla\rho}{2\rho}\right)^2 - \frac{\mathbf{v}^2}{2}$$

$$\mathbf{P}^{\mathrm{r}}_{\mathrm{SchM}} = -\frac{1}{8}\left(\Delta\rho\mathbf{I} + \nabla^2\rho - \frac{2\nabla\rho \otimes \nabla\rho}{\rho} \right)$$

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Potential form: $\nabla \cdot \mathbf{P}^{r} = \rho \nabla U_{Q}$

$\Psi = \sqrt{\rho} e^{-i\nabla \mathbf{v}}$

Bernoulli equation → Schrödinger equation

$$U_Q = -\partial_\rho(\rho s_e) + \nabla \cdot (\rho \partial_{\nabla\rho} s_e)$$

Euler-Lagrange form

Variational origin

Why nonequilibrium thermodynamics?

Thermodynamics $\neq$ science of temperature

Thermodynamics $\neq$ science of macroscopic energy changes

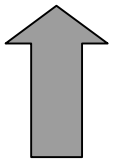
Thermodynamics (?) $=$ general framework of any macroscopic (?) continuum (?) theories

General framework:

- fundamental balances
- objectivity - frame indifference
- Second Law $\Rightarrow$ reversibility – special limit

Conclusions

- Not everything is a balance
- Second order nonlocality is interesting
- Constitutive entropy current
- Force-current systems: constructivity
- Variational principles



Second Law