Liu procedure: a method to solve the entropy inequality

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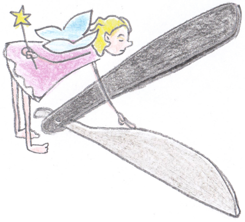
Content

Mathematics and physics

I.



II.

About the Second Law

Universalities and more

- Static part: existence of entropy as potential, dynamic part: entropy is increasing in real processes. (Constant entropy: ideal process.)
- Static universality. Absolute temperature: independent of material structure. Particles and radiation.
- Dynamic universality? Characteristic form of differential equations. Transport. Scaling properties.
- Static and dynamic parts: conditions of Lyapunov theorems. Material stability. Possibility of repeated experiments.
- Statistical mechanics cannot prove universal statements.
- Universal theories: gravity and quantum mechanics.

How to solve an inequality?

Pure dissipation: heat conduction in CIT

CIT = Classical Irreversible Thermodynamics.
The calculation of entropy production (Eckart, 1940):

$$\rho\dot{e} + \nabla\cdot\boldsymbol{q} = 0, \qquad de = Tds$$

$$\rho\dot{s} + \nabla\cdot\left(\frac{\boldsymbol{q}}{T}\right) = \frac{\rho\dot{e}}{T} + \nabla\cdot\left(\frac{\boldsymbol{q}}{T}\right) = \boxed{\boldsymbol{q}\cdot\nabla\frac{1}{T} \geq 0}$$

Solution of the inequality: $\boldsymbol{q}(e, \nabla e) = \lambda_T \nabla\frac{1}{T} = -\lambda\nabla T$, $\lambda(e) \geq 0$.

General aspects:

- spacetime: comoving derivative, constitutive state space,
- entropy: local thermodynamic potential,
- entropy inequality.

Material properties (statistical and kinetic origin):

- static EOS: $e = cT$,
- constitutive EOS?: $\boldsymbol{q} = -\lambda(e)\nabla T(e)$.

Hidden covariance

Spacetime aspects - separation of material and motion

$$\frac{\partial(\rho e)}{\partial t} + \nabla \cdot (\boldsymbol{q} + \rho \boldsymbol{v} e) = 0, \quad \rightarrow \quad \rho \dot{e} + \nabla \cdot \boldsymbol{q} = 0$$

It is a change of frame:

- comoving(substantial) time derivative: $\dot{e} = \frac{\partial e}{\partial t} + \boldsymbol{v} \cdot \nabla e$,
- balance of mass,
- convective and conductive current densities,
- total and internal energies: $e = e_{TOT} - v^2/2$.

Constitutive state space

Coleman-Noll and Liu procedures. Separation of functions and variables.
The entropy inequality is *conditional*:

$$\rho\dot{e} + \nabla\cdot\boldsymbol{q}(e,\nabla e) = 0,$$
$$\rho\dot{s}(e,\nabla e) + \nabla\cdot\boldsymbol{J}(e,\nabla e) - \Lambda(\rho\dot{e} + \nabla\cdot\boldsymbol{q}(e,\nabla e)) =$$
$$\rho\frac{\partial s}{\partial\nabla e}(\nabla e)^{\cdot} + \rho\left(\frac{1}{T}-\Lambda\right)\dot{e} + ... \geq 0$$

Liu-procedure, Lagrange–Farkas-multipliers. It follows that:

$$\frac{\partial s}{\partial\nabla e}(e,\nabla e) = 0, \qquad \Lambda = \frac{1}{T}, \quad \text{and} \quad \boldsymbol{q}(e,\nabla e)\cdot\nabla\left(\frac{1}{T}(e)\right) \geq 0$$

Constitutive state variables: $(e, \nabla e)$
$\rightarrow$ thermodynamic state variables: (e)
Process direction variables: $(\dot{e}, (\nabla e)^{\cdot}, \nabla^2 e)$

Farkas' lemma

Liu procedure: linear algebra and analysis.

Farkas(-Minkowski-Haar) lemma

If $\boldsymbol{a}_i \neq \boldsymbol{0}$, $i = 1, ..., n$ are vectors of a finite dimensional vector space $\boldsymbol{V}$ and $S = \{\boldsymbol{p} \in \boldsymbol{V^*} | \boldsymbol{p} \cdot \boldsymbol{a}_i \geq 0, i = 1, ..., n\}$ is a subset of the dual vector space, then the following staments are equivalent for all $\boldsymbol{b} \in \boldsymbol{V}$ vectors:
(i) $\boldsymbol{p} \cdot \boldsymbol{b} \geq 0$ for all $\boldsymbol{p} \in S$.
(ii) There exist $\lambda_1, ..., \lambda_n$ nonnegative real numbers, so that $\boldsymbol{b} = \sum_{i=1}^n \lambda_i \boldsymbol{a}_i$.
Remark:

$$\boldsymbol{p} \cdot \boldsymbol{b} - \sum_{i=1}^{n} \lambda_i \boldsymbol{p} \cdot \boldsymbol{a}_i = \boldsymbol{p} \cdot (\boldsymbol{b} - \sum_{i=1}^{n} \lambda_i \cdot \boldsymbol{a}_i) \geq 0, \quad \forall \boldsymbol{p} \in \boldsymbol{V}^*.$$

History:
Farkas proved it in his analysis of Fourier principle (of mechanics) in 1895 in Hungarian. Minkowski and Haar provided independent proofs later. The lemma is the base of the Bell inequalities and also the Karush-Kuhn-Thucker theorems of optimisation.

Evolution equations, variational derivatives

Scalar field evolution: $\dot\varphi = f(\varphi, \partial_i\varphi)$

$$\dot S(\varphi,\partial_i\varphi) - \lambda(\dot\varphi - f(\varphi,\partial_i\varphi)) = \underline{(\partial_\varphi S - \lambda)}\dot\varphi + \underline{\partial_{\partial_i\varphi} S}\,\partial_i\dot\varphi + \lambda f \geq 0$$

$$\partial_\varphi S - \lambda = 0, \quad \partial_{\partial_i\varphi} S = 0,$$

$$\boxed{0 \leq f\ \partial_\varphi S} \quad \to \quad f = l\ \partial_\varphi S, \quad (l \geq 0)$$

Extended approach: $\dot\varphi = f(\varphi, \partial_i\varphi, \partial_{ij}\varphi)$

- Higher order state space: $(\varphi, \partial_i\varphi, \partial_{ij}\varphi)$;
- Constitutive entropy flux;
- Gradient constraints: $\partial_i\dot\varphi = \partial_i f$

$$\dot S + \partial_i J^i - \lambda(\dot\varphi - f) - \Lambda^i(\partial_i\dot\varphi - \partial_i f) \geq 0$$

$$\partial_\varphi S = \lambda, \quad \partial_{\partial_i\varphi} S = \Lambda^i, \quad \partial_{\partial\varphi} S = 0$$

$$J^i = -\partial_{\partial_i\varphi} S\ f + \hat J^i(\varphi, \partial_i\varphi) \qquad \boxed{0 \leq f\,(\partial_\varphi S - \partial_i(\partial_{\partial_i\varphi} S))} = f\frac{\delta S}{\delta\varphi}$$

Korteweg fluids

Ván-Fülöp (Proc. Roy. Soc., 2004)
Ván-Kovács (Phil. Trans. Roy. Soc. A, 2020)

Korteweg fluids: history

Capillarity.
Van der Waals: gradient of density is a thermodynamic variable.
Korteweg (1905): second gradient of density, pressure expansion.

Balances of mass, momentum and internal energy:

$$\dot{\rho} + \rho \nabla \cdot \boldsymbol{v} = 0,$$
$$\rho \dot{\boldsymbol{v}} + \nabla \cdot \boldsymbol{P} = \boldsymbol{0},$$
$$(\rho \dot{e} + \nabla \cdot \boldsymbol{q} = -\boldsymbol{P} : \nabla \boldsymbol{v}.)$$

$$\boldsymbol{P} = \left(p - \alpha \Delta \rho - \beta (\nabla \rho)^2 \right) \boldsymbol{I} - \delta \nabla \rho \circ \nabla \rho - \gamma \nabla^2 \rho$$

$\alpha, \beta, \gamma, \delta$ are density dependent material parameters.

Violently instable. Second law? Eckart fluids (1948)!

Korteweg fluids – Liu procedure

Constitutive state variables: $(e, \nabla e, \rho, \nabla\rho, \nabla^2\rho, (\boldsymbol{v}), \nabla\boldsymbol{v})$

$\rightarrow$ thermodynamic state variables: $(e, \rho, \nabla\rho)$

Process direction: $(\dot{e}, (\nabla e)^\cdot, \nabla^2 e, \dot{\rho}, (\nabla\rho)^\cdot, (\nabla^2\rho)^\cdot, \nabla^3\rho, \dot{\boldsymbol{v}}, (\nabla^2\boldsymbol{v})^\cdot)$

$$\rho\dot{s} + \nabla\cdot\boldsymbol{J} = \boldsymbol{q}\cdot\nabla\left(\frac{1}{T}\right) -$$

$$-\left[\boldsymbol{P} - p\boldsymbol{I} - \frac{\rho^2}{2}\left(\nabla\cdot\frac{\partial s}{\partial\nabla\rho}\boldsymbol{I} + \nabla\frac{\partial s}{\partial\nabla\rho}\right)\right] : \frac{\nabla\boldsymbol{v}}{T} \geq 0$$

- Rigorous methods are essential.
- The pressure of an ideal, non-dissipative Korteweg fluid:

$$\boxed{\boldsymbol{P} = p(e,\rho)\boldsymbol{I} + \frac{\rho^2}{2}\left(\nabla\cdot\frac{\partial s}{\partial\nabla\rho}\boldsymbol{I} + \nabla\frac{\partial s}{\partial\nabla\rho}\right)}$$

Korteweg fluids – quantum mechanics

$$\boldsymbol{P_q} = \frac{\rho^2}{2}\left(\nabla \cdot \frac{\partial s}{\partial \nabla \rho}\boldsymbol{I} + \nabla \frac{\partial s}{\partial \nabla \rho}\right)$$

- 'Holographic' property:

$$\boxed{\nabla \cdot \boldsymbol{P_q} = \rho \nabla \phi}, \quad \text{whre} \quad \phi = \nabla \cdot \frac{\partial(\rho s)}{\partial \nabla \rho} - \frac{\partial \rho s}{\partial \rho} = -\delta_\rho(\rho s)$$

- Momentum balance: continuum AND point mass

$$\rho \dot{\boldsymbol{v}} + \nabla \cdot \boldsymbol{P_q} = \rho(\dot{\boldsymbol{v}} + \nabla \phi) = 0 \quad \rightarrow \quad \dot{\boldsymbol{v}} = -\nabla \phi$$

- Mass scale independent quadratic free energy → general Gross-Pitaevskii equation

$$s(e, \rho, \nabla \rho) = s_Q\left(e - \frac{\hbar^2}{2m}\frac{(\nabla \rho)^2}{4\rho^2}\right) \rightarrow \boxed{m\dot{\boldsymbol{v}} = -\nabla\left(\frac{\hbar^2}{2}\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}}\right)}$$

Bohm potential → inverse Madelung transformation → nonlinear Schrödinger equation

Newtonian gravity

Ván-Abe (Physica A, 2022)
Abe-Ván (arXiv:2205.05170, 2022)

Scalar field and hydrodynamics

$s(e - \varphi - \frac{\nabla\varphi\cdot\nabla\varphi}{8\pi G\rho}, \rho)$. Gibbs relation:

$$du = Tds + \frac{p}{\rho^2}d\rho = de - d\left(\varphi + \frac{\nabla\varphi\cdot\nabla\varphi}{8\pi G\rho}\right).$$

The potential energy, φ, the field energy and internal energy are separated.

Balances of mass, momentum, internal energy + field equation:

$$\dot{\rho} + \rho\nabla\cdot\boldsymbol{v} = 0,$$
$$\rho\dot{\boldsymbol{v}} + \nabla\cdot\boldsymbol{P} = \boldsymbol{0},$$
$$\rho\dot{e} + \nabla\cdot\boldsymbol{q} = -\boldsymbol{P} : \nabla\boldsymbol{v}.$$

Entropy inequality:

$$\boxed{\rho\dot{s} + \nabla\cdot\boldsymbol{J} = \Sigma \geq 0}$$

Gravity

Constitutive state variables: $(e, \nabla e, \rho, \nabla\rho, (\boldsymbol{v}), \nabla\boldsymbol{v}, \varphi, \nabla\varphi, \nabla^2\varphi)$

$\rightarrow$ thermodynamic state variabless: $(e, \rho, \varphi, \nabla\varphi)$

$$\rho\dot{s} + \nabla\cdot\boldsymbol{J} =$$

$$\left(\boldsymbol{q} + \frac{\dot{\varphi}}{4\pi G}\nabla\varphi\right)\cdot\nabla\left(\frac{1}{T}\right)$$

$$+\boxed{\frac{\dot{\varphi}}{4\pi G T}\left(\Delta\varphi - 4\pi G\rho\right)}$$

$$-\left[\boldsymbol{P} - p\boldsymbol{I} - \frac{1}{4\pi G}\left(\nabla\varphi\nabla\varphi - \frac{1}{2}\nabla\varphi\cdot\nabla\varphi\boldsymbol{I}\right)\right] : \frac{\nabla\boldsymbol{v}}{T} \geq 0$$

- Holographic property,
- Dissipative AND nondissipative together, without variational principles.

  Field equation:

$$\boxed{\frac{\tau}{l^2}\dot{\varphi} = \Delta\varphi - 4\pi G\rho - K\nabla\varphi\cdot\nabla\varphi.}$$

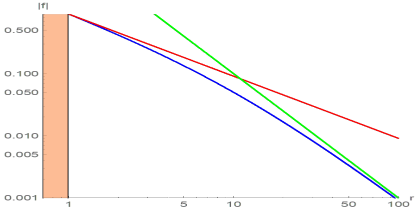
$$\boxed{0 = \Delta\varphi - 4\pi G\rho - K\nabla\varphi\cdot\nabla\varphi.}$$

Vacuum solutions $\rho = 0$:

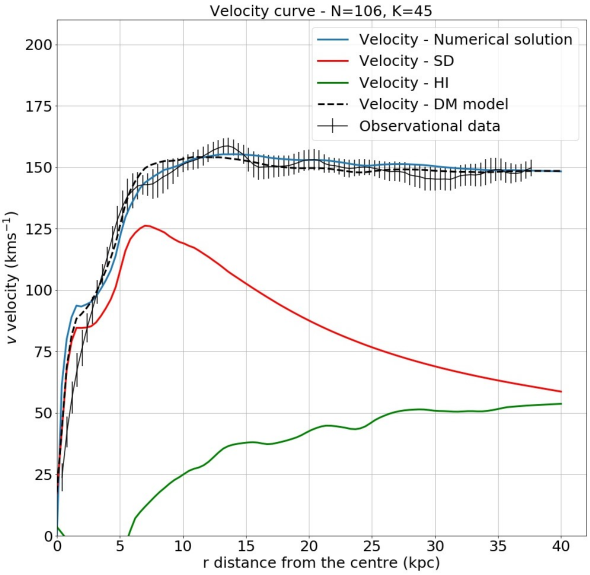
$$\varphi(\boldsymbol{r}) = \frac{1}{K}\ln(r)$$

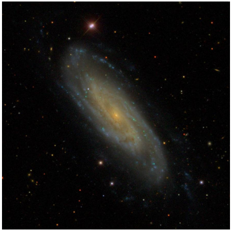
Spherical symmetric force field. Crossover. Apparent and real masses:

$$f(r) = -\frac{r_1}{Kr(r+r_1)} = -\frac{GM}{r(r+r_1)}$$



Modified gravity and Dark Matter





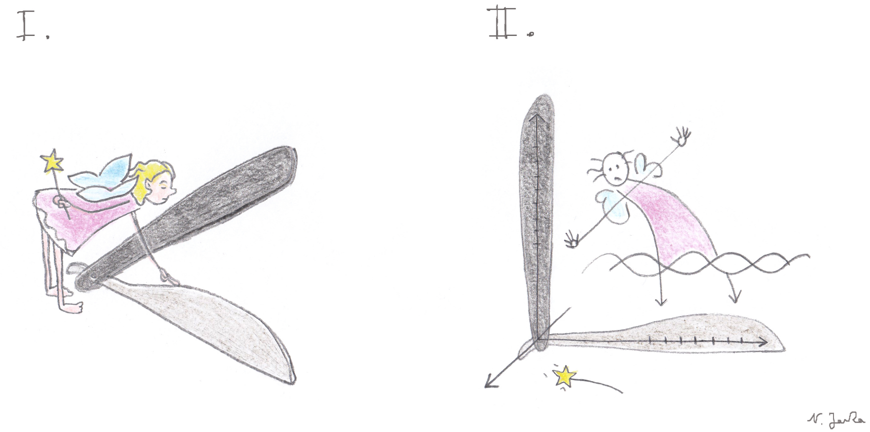
NGC 3198

Thanks to M. Pszota

Summary and notes

Nonequilibrium thermodynamics

- Thermodynamics $\neq$ statistical physics.
- Direct, rigorous, analytical methodology: Liu procedure.
- Universal dynamics. Compatibility tests: Newtonian gravity and quantum mechanics.
- Euler-Lagrange equations without variational principles.
- A uniform derivation of ideal and dissipative evolution equations.
- Long-range are local.



"This may be true, because it is mathematically trivial."
(somebody from Princeton, according to R. Pisarski)

Thank you for the attention!

Classical gradient expansions

Classified by constitutive state spaces and constraints

- Heat conduction. Internal energy or temperature. $(e, \partial_i e, \partial_{ij} e, ...)$.
  Constraint: balance of internal energy.
- Internal variables (e.g. phase fields). $(\varphi, \partial_i \varphi, \partial_{ij} \varphi, ...)$. Tensorial order may be arbitrary.
  Constraint: evolution equation, free or balance (Ginzburg-Landau-Alen-Cahn, Cahn-Hilliard).
- Fluid mechanics. Mass, velocity and energy. $(\rho, \partial_i \rho, \partial_{ij} \rho, v^i(?), ...))$, + more gradients.
  Constraints: balances of mass, momentum and energy.
- Solid mechanics. Mass, strain and energy $(\varepsilon^{ij}, \partial_k \varepsilon^{ij}, \partial_{kl} \varepsilon^{ij}, ...)$, and more gradients.
  Constraints: kinematics, balances of mass, momentum and energy.

General requirements: second law and objectivity.

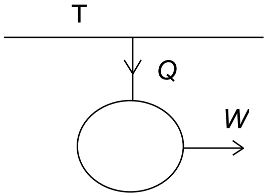
Equilibrium thermodynamics or thermostatics

Absolute temperature: does not depend on the material and the method of the measurement. It is not the scale, not the zero point, it is the *concept*. (Lord Kelvin, 1848. See e.g. Kardar, 2007).

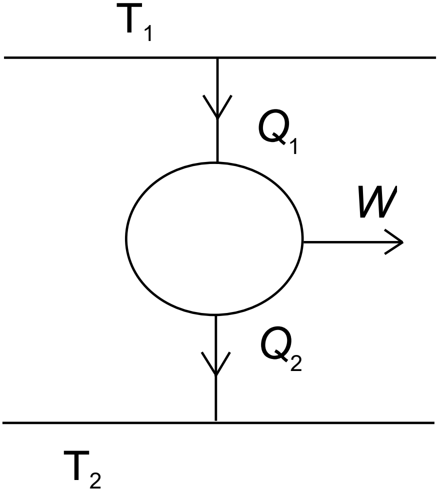
Kelvin-Planck form of the second law

It is impossible to devise a cyclically operating device, the sole effect of which is to absorb energy in the form of heat from a single thermal reservoir and to deliver an equivalent amount of work.

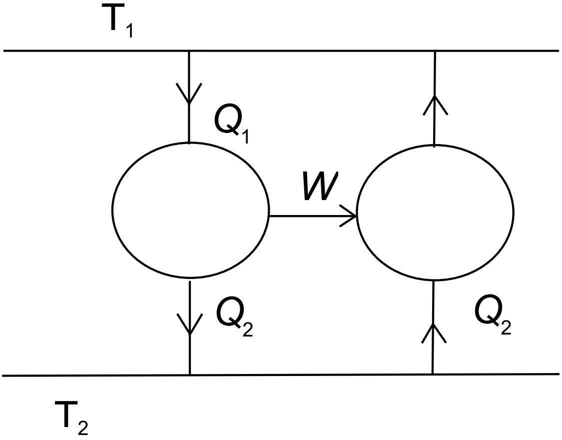
A perpetuum mobile of second kind:



A heat engine. Absorbs and emits heat and produces work.

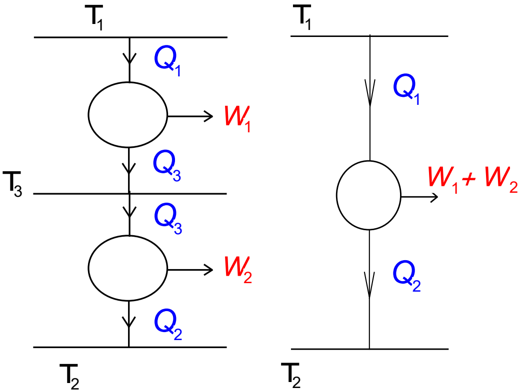


The reversible device is the most effective:



Efficiency depends only on the reservoir temperatures: $\eta(T_H, T_L)$

More heat engines:



Properties of efficiency:

$$\eta_1(T_1, T_3)\eta_2(T_3, T_2) = \eta_3(T_1, T_2) \quad \rightarrow \quad \eta(T_1, T_2) = \frac{\phi(T_1)}{\phi(T_2)} \quad \rightarrow \quad T = \frac{1}{\phi}.$$

Conditions: reversible process and the Kelvin-Planck form.

Variational principles for dissipative processes

Condition: symmetry

$$\boxed{\hat{\Theta}(\varphi) = 0}, \qquad \exists F : Dom(\hat{\Theta}) \to \mathbb{R}, \quad \delta F(\varphi) = \hat{\Theta}(\varphi)$$

δ derivation in a Banach (or Frechet) spaces, boundary conditions, ...

Necessary condition: $\hat{\Theta}$ is symmetric.

Many different variational principles

- Potentials: $\hat{\Theta} \circ \hat{\varphi}(\varphi) = 0$, where $\hat{\Theta} \circ \hat{\varphi}$ is symmetric
- Integrating multipliers: $\hat{T} \circ \hat{\Theta} = 0$, where $\hat{T} \circ \hat{\Theta}$ is symmetric
- Change the operator: $(\hat{\Theta}(\varphi))^2 = 0$, and neglect parts
- Change the function space: Gyarmati principle, ...,

All of them are right, which one is the true?

Connecting hydro to quantum

Gross-Pitaevskii equation:

$$i\hbar\frac{\partial\psi}{\partial t} + \frac{\hbar^2}{2m}\Delta\psi + \mu_0\psi - g\left|\psi\right|^2\psi = 0$$

μ_0 chemical potential, g interaction parameter ($\sim$ S-wave scattering length).
Madelung transformation:

$$\psi = \sqrt{\rho}e^{i\varphi},$$

ρ density (probability or superfluid), φ velocity potential: $\boldsymbol{v} = \frac{\hbar}{m}\nabla\varphi$.

$$\frac{i\hbar}{2\rho}\left(\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\boldsymbol{v})\right)\psi - \left(m\frac{\hbar}{m}\frac{\partial\varphi}{\partial t} + m\frac{v^2}{2} - \frac{\hbar^2}{2m}\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}} - \mu_0 + g\rho\right)\psi = 0$$

Continuity and Bernoulli equations of classical rotation free fluids. Its gradient will be:

$$m\dot{v} + \nabla(\mu_0 - g\rho + U_Q) = 0$$

$U_Q(\rho, \nabla\rho, \nabla^2\rho)$ is the Bohm potential. Special momentum balance.