

Entropy and Energy*

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Guiding question: how are energy and entropy related in macroscopic systems?

What you should look for in this talk:

- Mathematical theories of thermodynamics
- The tension between entropy and energy: why is thermodynamics confusing for a mathematician?
- What threads to pull on to study this topic further
- Future directions for the formalization of open thermodynamical systems using category theory

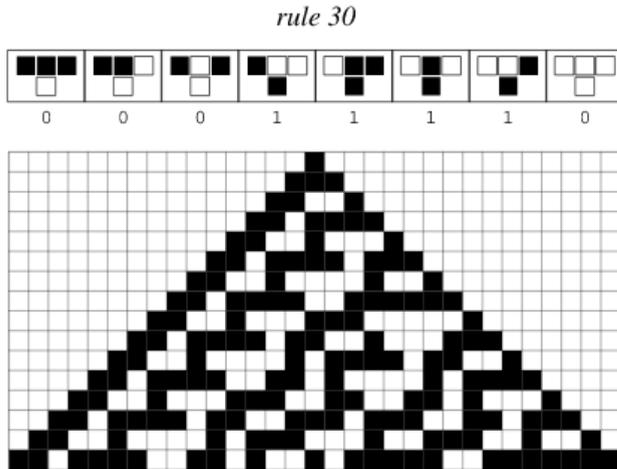
Today, the most exciting physics is not fundamental physics.

–John Baez [1]

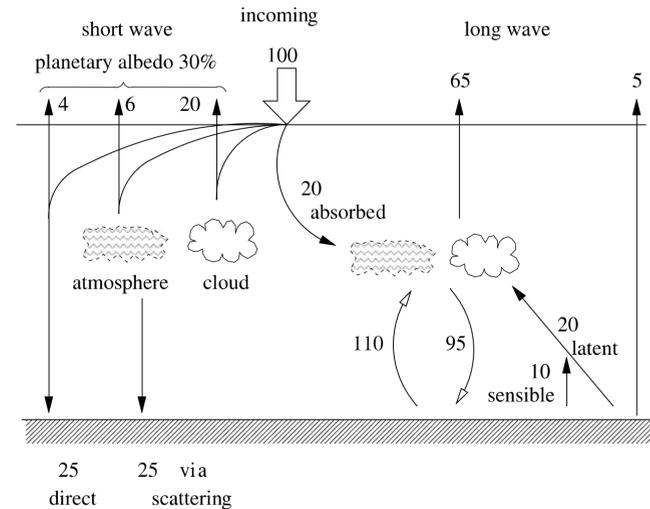
- 20th century: fundamental physics
 - Transistor (quantum mechanics) enables information revolution
 - Hydrogen bomb (nuclear physics) changes warfare forever
 - GPS (general relativity) obsoletes asking for directions
- 21st century: scale up to complex systems
 - Need to do ecology well in order to save planet
 - Need to engineer infrastructure to feed, house, and transport 8 billion people
 - Need to understand human body to cure diseases

Two ways that systems can be complex:

1. Systems can exhibit emergent behavior from simple rules.
2. Systems can be very complicated to specify.



Type 1 (Rule 30, [2])



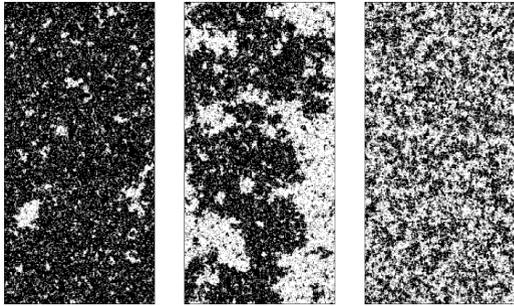
Type 2 (Solar radiation model, [3])

Figure 1. Type 1 vs. Type 2 complexity

We need to deal with both types of complexity.

Dealing with type 1 complexity means discovering *scientific properties* of systems, to enable new predictions

Example 1. Phase transition in lattice models. [4]



Dealing with type 2 complexity means building *formal structures* to model systems, to enable new abstractions

Example 2. Define a resource sharing machine [5] on an interface Y to be

- A space X
- A vector field $v: X \rightarrow TX$
- A resource-exposing map $e: X \rightarrow Y$

Thermodynamics is a good test case for both types of complexity.

- Thermodynamics studies emergent behavior of systems with many degrees of freedom.
- Thermodynamics is used widely within engineering disciplines to model complicated macroscale behavior.

Also:

Every mathematician knows it is impossible to understand an elementary course in thermodynamics.

– Vladimir Arnold [6]

Challenge accepted!

1. Energy in the driver's seat (Hamiltonian mechanics)
2. Entropy in the driver's seat (Entropy maximization)
3. Nobody in the driver's seat (Quasi-static processes, contact geometry)
4. Open systems (linear irreversible thermodynamics, port-Hamiltonian systems)
5. Entropy and Energy driving together (Exergy, GENERIC)

Hamiltonian mechanics in 3 easy steps: [7]

1. Find coordinates (q, p) for your system
2. Find total energy $H(q, p)$
3. Solve diff eq.

$$\dot{q} = \frac{\partial H}{\partial p}$$
$$\dot{p} = -\frac{\partial H}{\partial q}$$

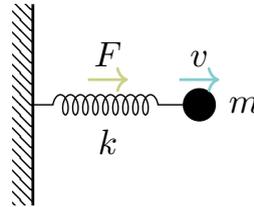


Figure 2. A mass on a spring

1. Coordinates: q is position, p is momentum
2. Energy

$$H(q, p) = \frac{1}{2m} p^2 + \frac{k}{2} q^2$$

3. Differential equations:

$$\dot{q} = \frac{\partial H}{\partial p} = \frac{p}{m}$$

$$\dot{p} = -\frac{\partial H}{\partial q} = -k q$$

More familiar as $\dot{x} = v$, $\dot{p} = F = -k x$.

Proposition 3. *Any solution of Hamilton's equations automatically conserves energy.*

Proof.

$$\frac{d}{dt}H(q(t), p(t)) = \langle dH(p(t), q(t)), (\dot{p}(t), \dot{q}(t)) \rangle = \frac{\partial H}{\partial q} \frac{\partial H}{\partial p} - \frac{\partial H}{\partial p} \frac{\partial H}{\partial q} = 0 \quad \square$$

“Energy is all you need”

A Poisson manifold X has precisely the structure necessary in order to make a vector field $v_H: X \rightarrow TX$ out of any scalar function $H: X \rightarrow \mathbb{R}$ such that

$$\nabla H \cdot v_H = 0$$

This implies that the dynamics of v_H conserve energy!

In quantum mechanics, the Hamiltonian is a self-adjoint operator on a Hilbert space, and we replace Hamilton's equations by the Schrodinger equation

$$\frac{d\psi}{dt} = -\frac{i}{\hbar} H\psi$$

These dynamics also conserve energy.

Conclusion: energy-driven systems have nice mathematics!

Equilibrium points of thermodynamical systems are found at maxima of the entropy with respect to constraints.

Example 4. Pie and icecream (continued on next slide)

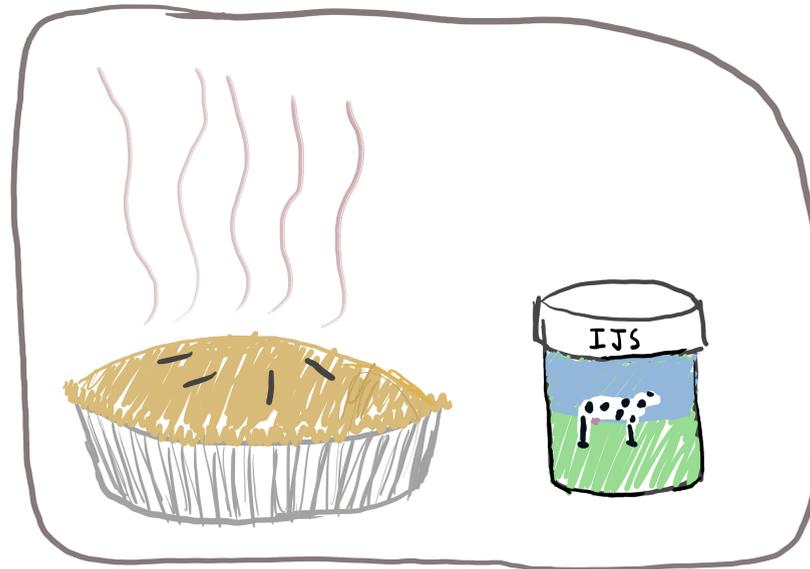


Figure 3. A hot pie and cold ice cream in an insulated container

This perspective formalized in [8].

- Model pie and ice cream as two thermal systems with heat capacities C_1, C_2

$$C_i T_i = U_i$$

- Entropy of each system given in terms of internal energies U_1, U_2 as

$$S_i(U_i) = C_i \log U_i$$

- Maximize $S_1(U_1) + S_2(U_2)$ subject to $U_1 + U_2 = U_{\text{tot}}$, where U_{tot} is fixed, we get

$$S_{\text{tot}}(U_{\text{tot}}) = \max_{U_1 + U_2 = U_{\text{tot}}} S_1(U_1) + S_2(U_2) = (C_1 + C_2) \log U_{\text{tot}} + \text{const}$$

- The overall system has the entropy function of a thermal system with heat capacity $C_1 + C_2$.
- Entropy maximization predicts temperature equalization between the two systems at equilibrium, where temperature is defined by

$$\frac{1}{T} = \frac{\partial S}{\partial U}$$

- Heat bath at temperature T :

$$S_{\text{bath}}(U) = \frac{U}{T}$$

- Probabilistic system of microstates i :

$$S_{\text{sh}}(p) = - \sum_i p_i \log p_i$$

- Maximize $S_{\text{sh}}(p) + S_{\text{bath}}(U)$ subject to condition that average energy is taken out of the heat bath.

$$\sum_i H_i p_i + U = 0$$

- Result is canonical ensemble

$$p_i = \frac{e^{-\frac{1}{T}H_i}}{\sum_i e^{-\frac{1}{T}H_i}}$$

- Quasi-static processes investigate paths of equilibria.
- How can a system have multiple equilibria?
- Equilibria depends on external conditions, external forces move system between equilibria
- First law:

$$dU = \bar{d}Q + \bar{d}W$$

- For an ideal gas:

$$dU = TdS - pdV$$

- What is this mathematically?

- A 1-form ω is a section of the cotangent bundle T^*X
- Can be integrated along a path $\gamma: [0, 1] \rightarrow X$ via

$$\int_{\gamma} \omega = \int_0^1 \omega_{\gamma(t)}(\gamma'(t)) dt$$

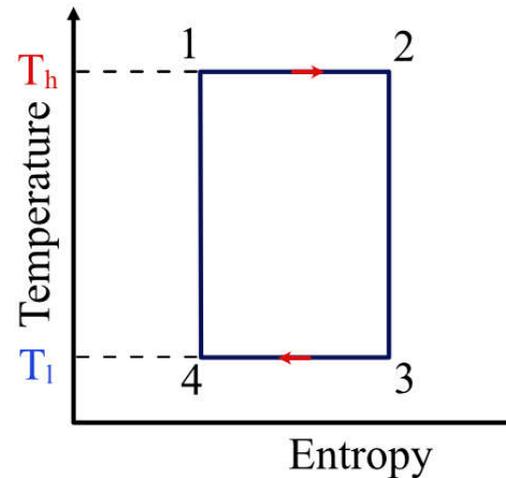
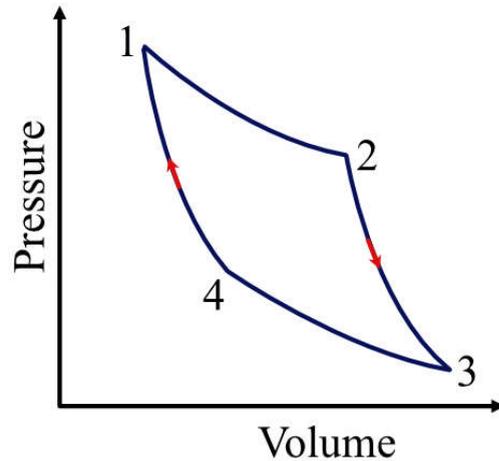
- A scalar function $f: X \rightarrow \mathbb{R}$ induces a gradient 1-form df
- 1-forms can be multiplied by scalar functions
- Let $X = \mathbb{R}^5$, with (U, S, V, T, p) the coordinate functions
- $\alpha = dU - T dS + p dV$ is a 1-form
- A material is described by a 2-dimensional surface of equilibria points $S \subset X$ such that α restricted to the tangent bundle $TS \subset TX$ is zero.
- Moving between equilibria is energy-conserving.
- Materials as surfaces resolves question of “what is a function of what?”

Definition 5. *Thermodynamic cycles are closed paths in the surface that defines a material.*

Example 6. Carnot cycle [9]

1-2 : Isothermal expansion
2-3 : Adiabatic expansion

3-4 : Isothermal compression
4-1 : Adiabatic compression



Carnot Cycle

Figure 4. Two different projections of a single closed path in \mathbb{R}^5

- Temperature, volume and pressure can be measured, energy and entropy cannot
- Pressure and temperature are intensive variables, energy, entropy, and volume are all extensive
- Energy and volume are properties of “microstates” (in the statistical mechanics interpretation) while pressure, temperature, and entropy are only properties of “macrostates”
- All quantities have different units
- It’s weird to have these very different quantities as coordinates for a manifold.
- Energy and entropy are functions of state in both Hamiltonian mechanics and entropy-maximization, but here they are part of the coordinates of the state.
- So how does thermodynamics relate to dynamical systems?

- Non-equilibrium thermodynamics sounds scary
- Actually some parts are very familiar
- The simplest type of non-equilibrium thermodynamics is linear irreversible [10]
 - Resistors
 - Diffusion
 - Friction
 - Newton's law of cooling
- Described (mutatis mutandis) by

$$I_{21} = \frac{1}{R}(V_2 - V_1)$$

- For resistors, diffusion, or friction the excess energy becomes heat
- For cooling, transfer of heat from hot to cold increases entropy
- Resistor networks studied in [11]

How can we construct a circuit with a resistor, capacitor, and inductor via composition?

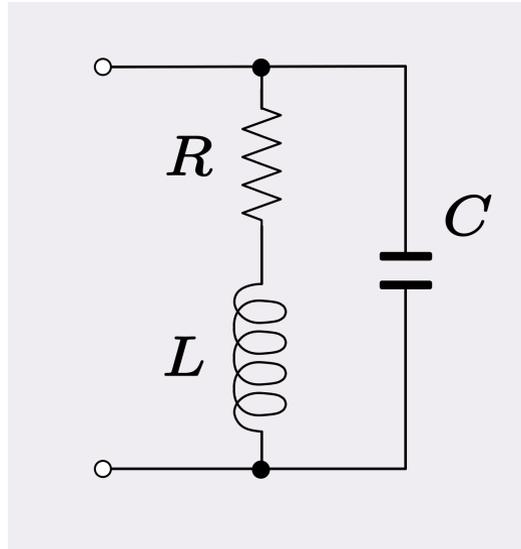


Figure 5. An RLC Circuit

End result should be damped oscillator.

$$\dot{q} = \frac{\Phi}{L}$$

$$\dot{\Phi} = \frac{q}{C} - \frac{\Phi R}{L}$$

Port-Hamiltonian systems are open systems whose interface consists of paired effort and flow

Domain	Effort	Flow
Electrical	Voltage	Current
Linear Mechanical	Force	Velocity
Rotational Mechanical	Torque	Angular Velocity
Hydraulic	Pressure	Volume flow
Thermal	Temperature	Entropy flow
Chemical	Chemical potential	Mass flow

Table 1. Effort and flow in various domains

Here are capacitors in different domains:

System	State variable	Constant	Effort	Flow
Capacitor	Charge (q)	Capacitance (C)	Voltage ($V = \frac{1}{C} q$)	Current ($I = \dot{q}$)
Lin. Spring	Length (x)	Compliance (C)	Force ($F = \frac{1}{C} x$)	Velocity ($v = \dot{x}$)
Coil Spring	Rotation (θ)	Ang. Compliance (C)	Torque ($\tau = \frac{1}{C} \theta$)	Ang. vel. ($\omega = \dot{\theta}$)
Inductor	Magnetic flux (Φ_B)	Inductance (L)	Current ($I = \frac{1}{L} \Phi_B$)	Voltage ($V = \dot{\Phi}_B$)
Particle	Momentum (p)	Mass (m)	Velocity ($v = \frac{1}{m} p$)	Force ($F = \dot{p}$)
Gyroscope	Ang. mmtm. (L)	Moment of Inertia (I)	Ang. vel. ($\omega = \frac{1}{I} L$)	Torque ($\tau = \dot{L}$)

Table 2. Systems analogous to capacitors

Port-Hamiltonian systems are built by composing generalized capacitors and generalized resistors in a bond-graph like syntax. [12]

Category-theory based composition for just “generalized capacitors” in master’s thesis [13]

- Traditional port-Hamiltonian systems have “dissipative components” (i.e. resistors), but don’t consider entropy explicitly.
- One way to work with energy and entropy is to combine them into an “exergy” potential:

$$B = U + pV - TS$$

Physically, this is defined to be “the energy that can be extracted from the system to do useful work”

- In [14], Exergetic Port-Hamiltonian Systems are developed
- Downside is that you need reference pressure/temperature/chemical potential/voltage etc.

- Another way is the “two-potential” approach, called GENERIC (General Equation for Non-Equilibrium Reversible-Irreversible Coupling)
- State space X with $E, S: X \rightarrow \mathbb{R}$. Then

$$\frac{dx}{dt} = L(x) \frac{\delta E}{\delta x} + M(x) \frac{\delta S}{\delta x}$$

where $L(x)$ is a “Poisson matrix” and $M(x)$ is a “friction matrix”. When $M(x) = 0$, this is just Hamilton’s equations for a Poisson manifold.

- Here, finally, entropy and energy are both driving!
- A resistor here is modeled as energy conserving; it converts electrical energy into heat energy
- I don’t yet know how to make the “open systems” version of GENERIC

- In classical mechanics and quantum mechanics, everything is “driven by energy”, via Hamilton’s and Schrodinger’s equations. Moreover, systems are typically closed/isolated.
- In equilibrium thermodynamics/statistical mechanics, everything is “driven” by entropy maximization, and often “open” in the sense that they are connected to a heat bath.
- Three approaches to irreversibility in non-equilibrium thermodynamics:
 - Dissipative structures (i.e. linear irreversible thermodynamics), just forget about the energy which dissipates
 - Exergy-based systems, which account for what portion of their energy is useful, but rely on reference intensive quantities
 - GENERIC systems, which use a double-potential system to model dynamics due to energy and due to entropy simultaneously
- Currently, with category theory I can compose
 - Entropy maximizers
 - Reversible port-Hamiltonian systems
- Lots more work to do!

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