Deriving Thermodynamics from Linear Dissipativity Theory

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

  (V. I. Arnold, 1990)

- In this talk: we keep trying
- Specifically: derive Fourier’s law from linear microscopic dynamics
- Key tools:
  - Dissipativity
  - Port-Hamiltonian systems

Thermodynamics

- A phenomenological theory of how heat flows/transforms
- Fourier's law (1822): $q_{\text{hot-to-cold}} = k(T_{\text{hot}} - T_{\text{cold}})$
- Carnot, Clausius, Kelvin (>1824): entropy, free energy, etc. as Lyapunov functions for isolated, constant-temperature, etc. systems
- Variables: internal energy, volume, temperature, etc. = macroscopic variables
- Not derived from atomic theory but from macroscopic observations

Microscopic foundations for thermodynamics

- Boltzmann, Maxwell, Gibbs (>1866)
- Hamiltonian, lossless microscopic dynamics
- Random micro state
- Macro state = probability measure on the micro state, parametrized by macro variable
- Entropy = Shannon entropy of micro state given macro state
- **But:**
  - Lack of complete and rigorous derivation of thermodynamics from micro dynamics
  - Little use of control theory (e.g. port-Hamiltonian systems) by stat. phys., while thermodynamics is a theory of open systems

A story of thermodynamics from control-theoretic point of view

- **This talk**: recover basic facts of thermodynamics
- No new physical content
- Use language of control theory, e.g. Willems's dissipativity theory
- Focus on linear systems
- Focus on recovering Fourier's law and introducing a new Lyapunov function

Microscopic systems are lossless

- A microscopic system is of the form

$$\dot{x}(t) = Ax(t) + Bu(t)$$
$$y(t) = B^T x(t)$$

with

  - state x
  - input (e.g. forces, voltages) u
  - output (e.g. speeds, currents) y
  - power into system $u^T y$
  - Energy = Hamiltonian $H = \frac{1}{2} x^T x$
  - Skew symmetry $A + A^T = 0$
- Lossless port-Hamiltonian system
- Energy is preserved

Macroscopic systems are dissipative

- Limits of very high-dim lossless systems =

(low-dim) dissipative systems. Cf. Sandberg-Delvenne-Doyle (TAC, 2011)

- Example: ideal resistance = infinite-dim lossless transmission line

- Thus macroscopic systems look dissipative:

$$\dot{x}(t) = (A - R)x(t) + Bu(t)$$
$$y(t) = B^T x(t)$$

- $R = R^T \succeq 0$ is the friction/resistance/dissipation term

Macroscopic system with noise

- Random high-dim micro initial condition becomes noise into low-dim dissipative model:

$$\dot{x}(t) = (A - \sum_j R_j)x(t) + Bu(t) + \sum_j \sqrt{2T_j R_j} w_j(t),$$

$$y(t) = B^T x(t),$$

where

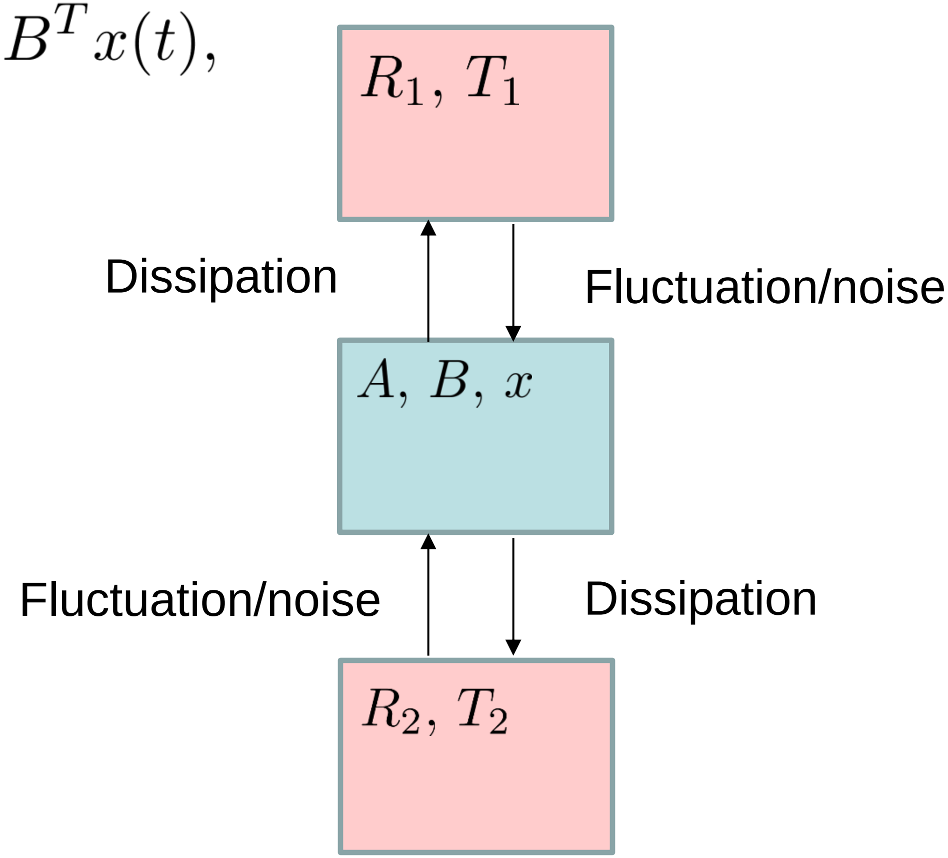
  - $w_j(t)$ = unit Gaussian white noise for resistance j
  - T_j = temperature of noise = thermal bath

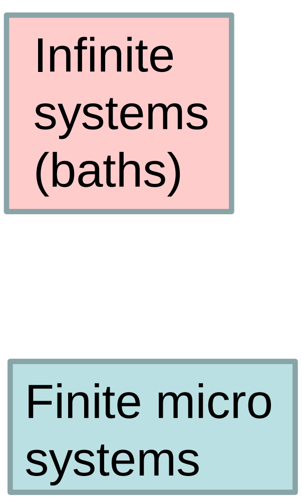
- Same resistance both in diss. and fluct. terms: = fluctuation-dissipation theorem
- Cf. Sandberg-Delvenne-Doyle (TAC, 2011)

Macroscopic system with noise

$$\dot{x}(t) = (A - \sum_j R_j)x(t) + Bu(t) + \sum_j \sqrt{2T_j R_j}\, w_j(t),$$

$$y(t) = B^T x(t),$$

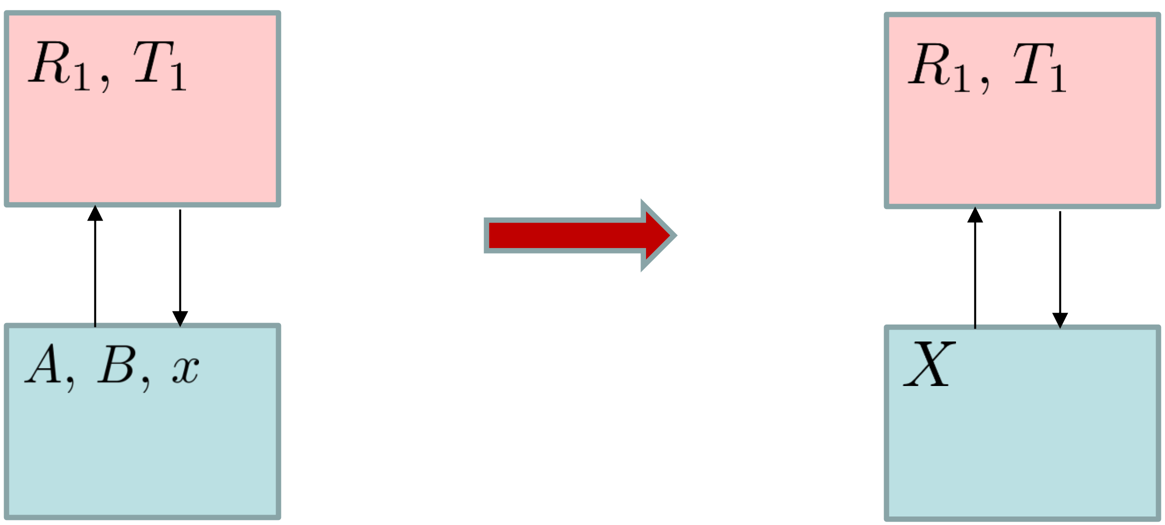




Thermodynamic state equation

- Assume centered Gaussians distributions for state (called Gibbs states)
- Deriving thermodynamics = finding dynamics of probability distributions
- Here state space = covariance matrix (« meta-state »)
- Thermodynamic state equation = Lyapunov equation

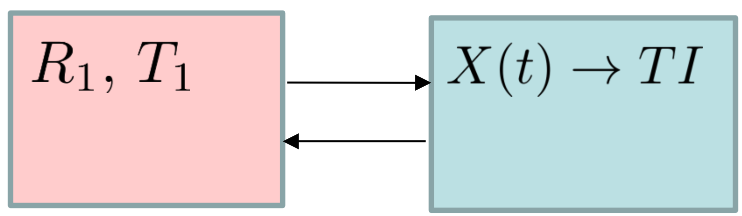
$$\dot{X} = AX + XA^T - \sum_j R_j X - \sum_j X R_j^T + 2 \sum_j R_j T_j$$



The state equation is dissipative

$$\dot{X} = AX + XA^T - \sum_j R_j X - \sum_j X R_j^T + 2 \sum_j R_j T_j$$

- Our contribution: observe the Lyapunov equation itself is a deterministic dissipative system with
  - storage function = « meta-energy » = $H_{\mathrm{meta}} = \frac{1}{2}\mathrm{Tr} X^2$
  - input = bath temperatures = T_j
  - output = power dissipated by resistances

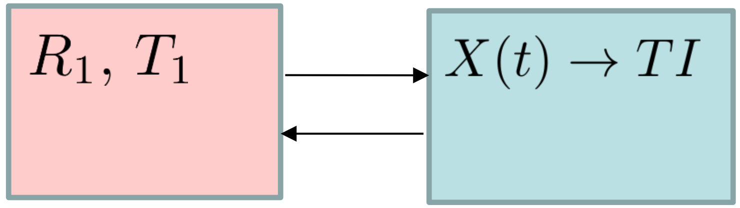


- Lyapunov function when single constant input temperature

$$H_{\mathrm{meta}} - 2T\mathbb{E}H$$

where $\mathbb{E}H$ is expected energy, so-called <u>internal energy</u>

Thermodynamics of one-bath systems



- Classical analysis: use free energy

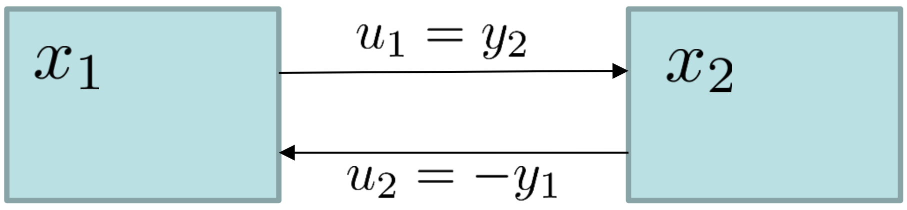
$$F = \mathbb{E}H - TS, \quad S = \int \rho \log \rho = \mathrm{Entropy}$$

as Lyapunov function to prove convergence to equilibrium (equipartition in linear case)

- Here we find « meta-energy » plays the role of entropy and seems more natural for linear systems
- Our Lyapunov function also generalizes to several constant input temperatures
- NB: Distinct from Haddad *et al*.'s ectropy (2008)

Fourier's law and the paradox of instant heat transfer

- Consider two micro systems



- If $x_1(0) \perp\!\!\!\perp x_2(0)$, the instant energy transfer

$$\mathbb{E} y_1 y_2 = \operatorname{Tr} C_1^T C_2 X_{12}$$

is zero, against Fourier's law

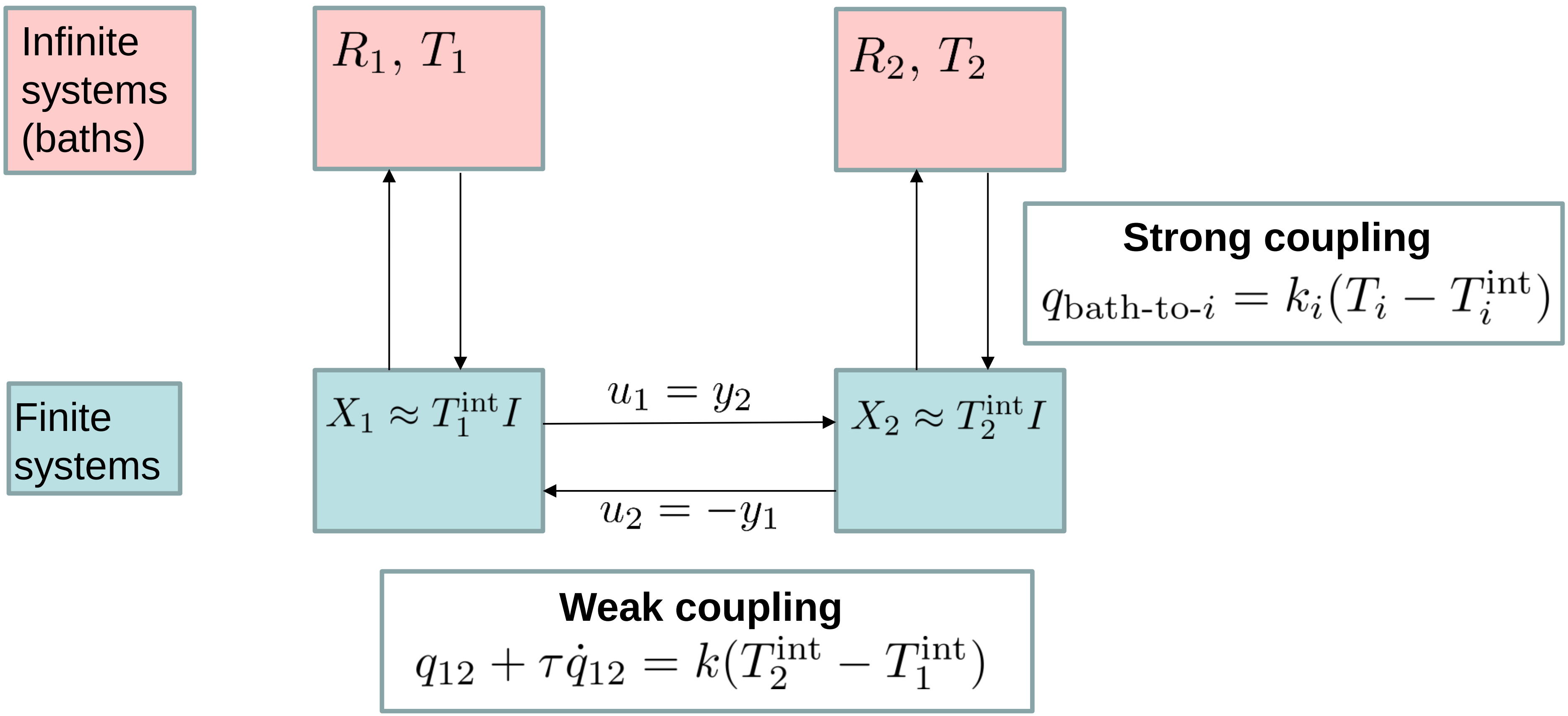
$$q_{12} = k(T_2 - T_1)$$

- How can we make Fourier's law compatible with our thermodynamics of linear systems?

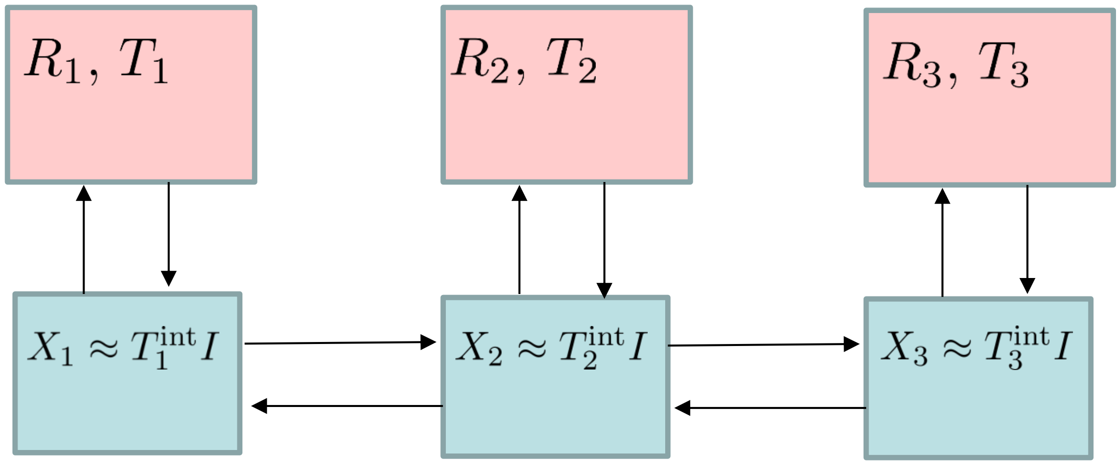
Maxwell-Cattaneo's law

- We assume:
  - Time scale separation: interaction between two systems slow compared to internal dynamics of systems (cf. Simon-Ando, 1961)
  - Local equilibrium: each system is close to equilibrium with a heat bath
- We find : $q_{12} + \tau \dot{q}_{12} = k(T_2 - T_1)$ where
  - τ is a relaxation time
  - k is thermal conductance
- = Maxwell-Cattaneo's law
- Classically introduced to avoid infinite propagation in parabolic heat equation
- Allows brief heat flow from cold to hot!

Maxwell-Cattaneo's law emerges from time scale separation



Network of systems



- Generalize to any network of systems
- Node has temperature, internal energy, total energy
- Edge has thermal conductivity, relaxation time
- Energy exchange through Fourier-Maxwell-Cattaneo's law
- We so recover Local Equilibrium Theory of non-equilibrium thermodynamics
- Also a justification of Haddad *et al*.'s phenomenological axioms (2008)

Conclusion

- Elementary derivation of classic results of thermodynamics from microscopic principles
  - Equipartition theorem
  - Fourier's law corrected to Maxwell-Cattaneo's law
- Dynamical systems tools:
  - dissipativity
  - port-Hamiltonian systems
  - time-scale separation
- New concept: meta-energy instead of entropy
- How to introduce work (e.g. pressure-volume, current-voltage) and Carnot's theorem: need nonlinear control: cf. Delvenne-Sandberg (Physica D, 2014)
- Extension to fully nonlinear systems?