Thermodynamics of Quantum Information Flows

Krzysztof Ptaszyński[1], Massimiliano Esposito[2]

[1]Institute of Molecular Physics, Polish Academy of Sciences, Poznań
[2] Complex Systems and Statistical Mechanics, University of Luxembourg

College on Energy Transport and Energy Conversion in the Quantum Regime

ICTP, August 26, 2019

Outline

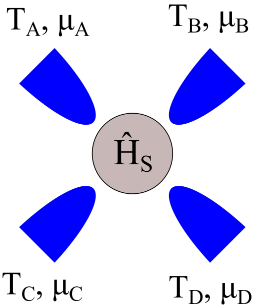
- Goal: Find thermodynamics constrains on information flows across an open Q-system
- 2nd law for open Q-systems
- Main result: local 2nd laws with information flows
- Previous works on Maxwell's demon
- Derivation of the main result
- Application to an autonomous Q-Maxwell demon

2nd law for open systems

$$\sigma = \Delta S - \sum_{\alpha} \beta_\alpha Q_\alpha \geq 0$$

where

- σ – entropy production
- S – entropy of the system
- Q_α – heat delivered from the reservoir α



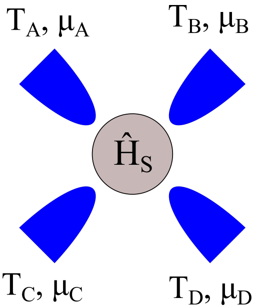
Markovian systems (weak coupling)

2nd law in differential form

$$\dot{\sigma} = d_t S - \sum_{\alpha} \beta_\alpha \dot{Q}_\alpha \geq 0$$

where

- $\dot{\sigma}$ – entropy production rate
- $S = -\mathrm{Tr}(\rho \ln \rho)$ – von Neumann entropy of the system
- $\dot{Q}_\alpha$ – heat flow from the reservoir α



[Spohn, Lebowitz, Adv. Chem. Phys. **38**, 109 (1978)]

Main result: local Clausius inequality

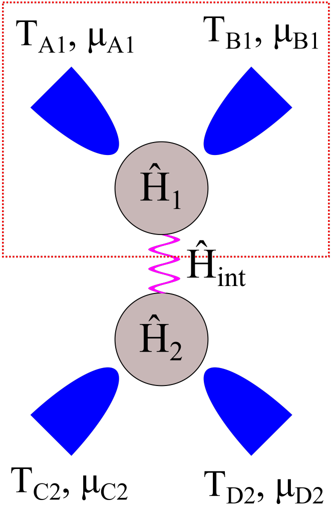
$$\hat{H}_S = \sum_i \hat{H}_i + \hat{H}_{\text{int}}$$

- Can we define 2nd law for a single subsystem? Yes!
- **Local Clausius inequality**

$$\dot{\sigma}_i = d_t S_i - \sum_{\alpha_i} \beta_{\alpha_i} \dot{Q}_{\alpha_i} \boxed{-\dot{I}_i} \geq 0$$

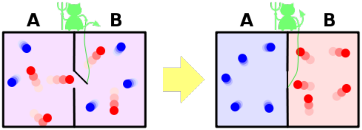
where

- $\dot{\sigma}_i$ – local entropy production rate
- $S_i = -\text{Tr}(\rho_i \ln \rho_i)$ – von Neumann entropy of the subsystem i
- $\dot{Q}_{\alpha_i}$ – heat flow from reservoir α_i
- $\dot{I}_i$ – information flow between the subsystems (defined later)



Maxwell demons

- Maxwell demon – entropy of a stochastic system can be reduced by a feedback control by an intelligent being



https://commons.wikimedia.org

- Experimental realizations
  - Molecular ring [Leigh group, Nature 445, 523 (2007)]
  - Single atoms [Raizen group, PRL 100, 093004 (2008)]
  - Colloidal particles [Sano group, Nat. Phys. 6, 988 (2010)]
  - Single-electron boxes [Pekola group, PRL 113, 030601 (2014)]
  - Superconducting circuits [Masuyama group, Nat. Com. 9, 1291 (2018)]

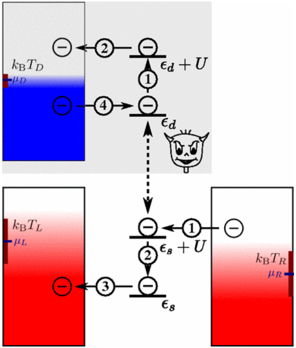
- 2nd laws with mutual information due to nonautonomous feedback
  - [Sagawa, Ueda, PRL 100, 080403 (2008)] (System only)
  - [Sagawa, Ueda, PRL 102, 250602 (2009)] (System + Memory)

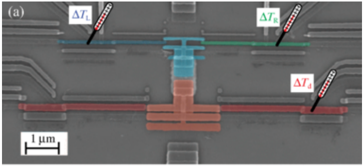
Autonomous Maxwell demons

- [Esposito, Schaller, EPL 99, (2012)] (System only)
- [Strasberg *et al.*, PRL 110, 040601 (2013)] (System + Demon)
- Experimental realization – [Koski *et al.*, PRL 115, 260602 (2015)]

No mutual information....

Connection between autonomous and nonautonomous was unclear



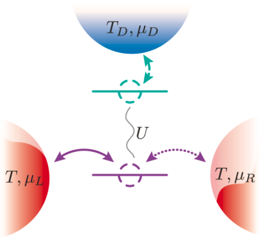


Unified framework within stochastic thermodynamics

- Two subsystems: X and Y
- Classical rate equation for state probabilities

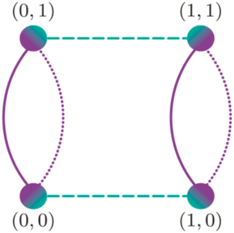
$$\dot{p}(x,y) = \sum_{x',y'} \left[W_{x,x'}^{y,y'} p(x',y') - W_{x',x}^{y',y} p(x,y) \right]$$

$W_{x,x'}^{y,y'}$ – rate of transition $(x',y') \to (x,y)$



- **Bipartite** transitions – either in X or Y, not simultaneous

$$W_{x,x'}^{y,y'} = \begin{cases} w_{x,x'}^{y} & x \neq x; y = y' \\ w_{x}^{y,y'} & x = x', y \neq y' \\ 0 & x \neq x', y \neq y' \end{cases}$$



[J. M. Horowitz, M. Esposito, Phys. Rev. X **4**, 031015 (2014)]

Local 2nd of thermodynamics

- Mutual information – measure of correlation between subsystems

$$I = H_X + H_Y - H = \sum_{x,y} p(x,y) \ln \frac{p(x,y)}{p(x)p(y)} \geq 0$$

where H is the Shannon entropy.

- Decomposition: $d_t I = \dot{I}_X + \dot{I}_Y$

$$\dot{I}_X = \sum_{x \geq x'; y} \left[w^y_{x,x'} p(x',y) - w^y_{x',x} p(x,y) \right] \ln \frac{p(y|x)}{p(y|x')}$$

- Local 2nd law

$$\boxed{\dot{\sigma}_i = \dot{H}_i - \beta_i \dot{Q}_i - \dot{I}_i \geq 0}$$

[J. M. Horowitz, M. Esposito, Phys. Rev. X **4**, 031015 (2014)]

Limitations

- Classical systems with bipartite structure

- Q-systems without eigenbasis coherences **and** satisfying $[\hat{H}_{\text{int}}, \hat{H}_i] = 0$

  Since rate equations describe transtions between eigenstates of the total Hamiltonian $\hat{H}_S$, the eigenstates of $\hat{H}_S$ must be products of eigenstates of subsystem Hamiltonians $\hat{H}_i$ for the transition matrix to have a bipartite structure

- **We will now** generalize the concept of autonomous information flow to a generic Markovian open Q-system

Derivation: Key ingredients

- Dynamics described by Lindblad equation

$$d_t\rho = -i\left[\hat{H}^{\text{eff}}, \rho\right] + \mathcal{D}\rho$$

- Additivity of dissipation – interaction with each reservoir gives an independent contribution to the dissipation

$$\mathcal{D} = \sum_{\alpha} \mathcal{D}_\alpha$$

- Local equilibration

$$\mathcal{D}_\alpha \rho_\alpha^{\text{eq}} = 0$$

$$\text{where} \quad \rho_\alpha^{\text{eq}} = Z_\alpha^{-1} e^{-\beta_\alpha\left(\hat{H}_S - \mu_\alpha \hat{N}\right)}$$

Partial Clausius inequality

- Applying Spohn's inequality [Spohn, J. Math. Phys. 19, 1227 (1978)]

$$-\mathrm{Tr}\left[(\mathcal{D}^\alpha \rho)\left(\ln \rho - \ln \rho^\alpha_{\mathrm{eq}}\right)\right] \geq 0$$

  one obtains the **partial Clausius inequality**

  [Cuetara, Esposito, Schaller, Entropy 18, 447 (2016)]

$$\boxed{\dot{\sigma}_\alpha = \dot{S}^\alpha - \beta_\alpha \dot{Q}_\alpha \geq 0}$$

  where

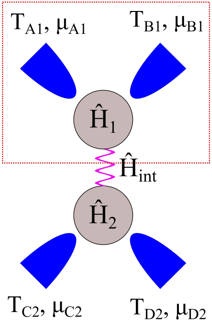
  - $\dot{\sigma}_\alpha$ – partial entropy production rate
  - $\dot{S}^\alpha = -\mathrm{Tr}\left[(\mathcal{D}^\alpha \rho) \ln \rho\right]$ – rate of change of the von Neumann entropy due to interaction with the reservoir α
  - $\dot{Q}_\alpha = \mathrm{Tr}\left[(\mathcal{D}^\alpha \rho)\left(\hat{H}_S - \mu_\alpha \hat{N}\right)\right]$ – heat flow from the reservoir α

- **Meaning**: interaction with each reservoir gives a non-negative contribution to the entropy production

Local Clausius inequality

$$\dot{\sigma}_\alpha = \dot{S}^\alpha - \beta_\alpha \dot{Q}_\alpha \geq 0$$

- Local entropy production rate – sum of $\dot{\sigma}_{\alpha_i}$ associated with reservoirs α_i coupled to subsystem i



$$\dot{\sigma}_i = \sum_{\alpha_i} \dot{\sigma}_{\alpha_i} = \sum_{\alpha_i} \dot{S}^{\alpha_i} - \sum_{\alpha_i} \beta_{\alpha_i} \dot{Q}_{\alpha_i} =$$

$$d_t S_i \underbrace{\boxed{-d_t S_i + \sum_{\alpha_i} \dot{S}^{\alpha_i}}}_{-\dot{I}_i} - \sum_{\alpha_i} \beta_{\alpha_i} \dot{Q}_{\alpha_i} \geq 0$$

- We obtain the Q-analogous the Horowitz-Esposito result

$$\boxed{\dot{\sigma}_i = d_t S_i - \sum_{\alpha_i} \beta_{\alpha_i} \dot{Q}_{\alpha_i} - \dot{I}_i \geq 0}$$

Q-Information flow

- Is the information flow, $\dot{I}_i$, related to mutual information? Yes!

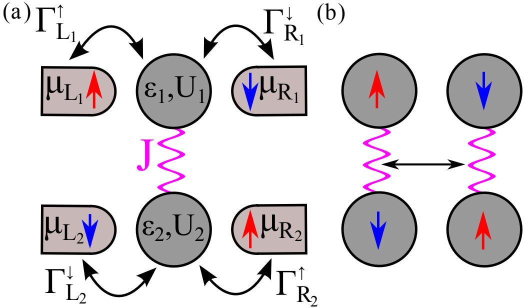
$$\sum_i \dot{I}_i = d_t I$$

where $I = \sum_i S_i - S$ is the (multipartite) Q-mutual information between the subsystems

- Using secular approximation with $[\hat{H}_{\text{int}}, \hat{H}_i] = 0$, we recover the Horowitz-Esposito result.

Application: Autonomous Q-Maxwell's demon

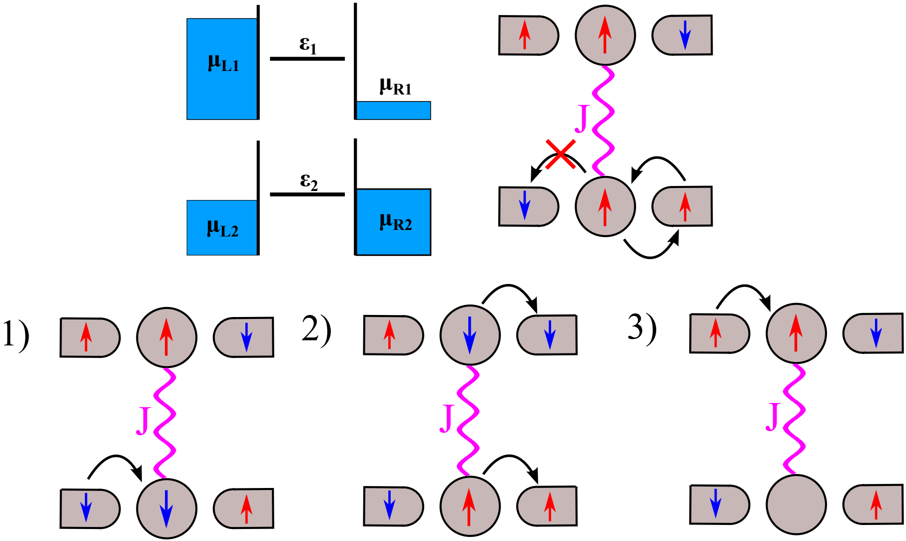
$$\hat{H}_S = \sum_{i\in\{1,2\}} \sum_{\sigma\in\{\uparrow,\downarrow\}} \epsilon_i c^\dagger_{i\sigma} c_{i\sigma} + \sum_{i\in\{1,2\}} U_i n_{i\uparrow} n_{i\downarrow} + J(\hat{S}^x_1 \hat{S}^x_2 + \hat{S}^y_1 \hat{S}^y_2)$$



K. Ptaszyński, Phys. Rev. E **97**, 012116 (2018)

- Operation based on coherent spin exchange + spin selective dissipative dynamics (next slide)
- Essentially non-bipartite dynamics: spin exchange simultaneously flip spins in both dots; $[\hat{H}_{\text{int}}, \hat{H}_i] \neq 0$
- Could not be described by previously existing approaches

Demon operation

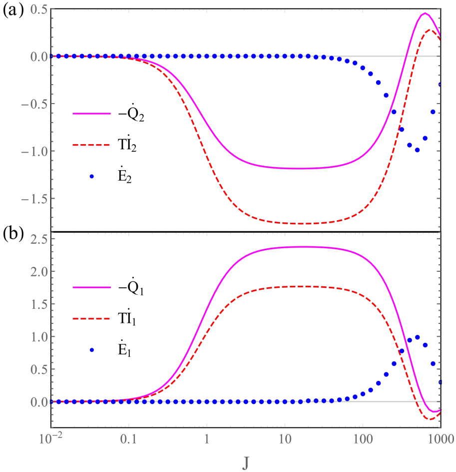


Results

$$T\dot{\sigma}_1 = -\dot{Q}_1 - T\dot{I}_1 \geq 0$$
$$T\dot{\sigma}_2 = -\dot{Q}_2 + T\dot{I}_1 \geq 0$$

because $\dot{I}_2 = -\dot{I}_1$

- $J \lessapprox 100$ is the "pure" Maxwell demon regime:
  - 2 is cooled ($\dot{Q}_2 > 0$)...
  - ...with a negligible energy flow $\dot{E}_i \approx 0$...
  - ...thanks to an information flow $T\dot{I}_1 > \dot{Q}_2$



$T = 100, \; V_1 = 60, \; V_2 = -30$

Conclusions

- We derived local 2nd laws with information flows for parts of a Markovian Q-systems coupled to several reservoirs
- This provides a consistent framework for thermodynamics of Q-information flows
- Applicability of our approach was demonstrated on the example of an autonomous Q-Maxwell demon

- More details: [K. Ptaszyński and M. Esposito, *Thermodynamics of Quantum Information Flows*, PRL **122**, 150603 (2019)]

Acknowledgments

- K. P. is supported by the National Science Centre, Poland, under the project Opus 11 (No. 2016/21/B/ST3/02160) and the doctoral scholarship Etiuda 6 (No. 2018/28/T/ST3/00154). M. E. is supported by the European Research Council project NanoThermo (ERC-2015-CoG Agreement No. 681456).

erc
European Research Council
Established by the European Commission

NATIONAL SCIENCE CENTRE
POLAND

Thank you for your attention!

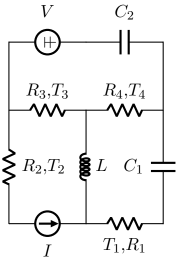
Stochastic and quantum thermodynamics of driven RLC networks

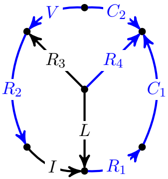
Nahuel Freitas, Jean-Charles Delvenne, Massimiliano Esposito

ICTP, Trieste

August 2019

Dynamics of RLC networks



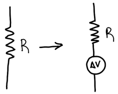


Deterministic dynamics:

$$\boxed{\frac{dx}{dt} = \mathcal{A}(t)\mathcal{H}(t)\,x + \mathcal{B}(t)s(t)}$$

$$x = \begin{bmatrix} q \\ \phi \end{bmatrix} \qquad s = \begin{bmatrix} v_E \\ j_I \end{bmatrix} \qquad \mathcal{H} = \begin{bmatrix} C^{-1} & \\ & L^{-1} \end{bmatrix}$$

Classical stochastic dynamics:



- $\langle \Delta v(t) \rangle = 0$
- $\langle \Delta v(t) \Delta v(t') \rangle = 2Rk_bT\,\delta(t-t')$

$$\boxed{\frac{dx}{dt} = \mathcal{A}(t)\mathcal{H}(t)\,x + \mathcal{B}(t)s(t) + \sum_r \sqrt{2k_bT_r}\,\mathcal{C}_r\,\xi(t)}$$

$$\langle \xi_i(t)\xi_j(t') \rangle = \delta_{i,j}\delta(t-t') \qquad (\mathcal{A})_s = \frac{\mathcal{A}+\mathcal{A}^T}{2} = -\sum_r \mathcal{C}_r\mathcal{C}_r^T$$

Stochastic thermodynamics of RLC networks

The mean values $\langle x \rangle$ and the covariance matrix $\sigma = \langle x x^T \rangle - \langle x \rangle \langle x \rangle^T$ evolve according to:

$$\frac{d\langle x \rangle}{dt} = \mathcal{A}\mathcal{H}(t)\,\langle x \rangle + \mathcal{B}(t)s(t) \qquad \frac{d}{dt}\sigma(t) = \mathcal{A}\mathcal{H}(t)\sigma(t) + \sigma(t)\mathcal{H}(t)\mathcal{A}^T + \sum_r 2k_b T_r\,\mathcal{C}_r\mathcal{C}_r^T$$

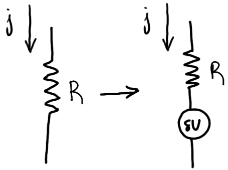
We can identify work and heat currents by analyzing the change of the circuit energy:

$$E = \frac{1}{2}x^T\mathcal{H}(t)x \qquad \Longrightarrow \qquad \langle E \rangle = \frac{1}{2}\,\mathrm{Tr}\left[\mathcal{H}(t)\langle x \rangle\langle x \rangle^T\right] + \frac{1}{2}\,\mathrm{Tr}\left[\mathcal{H}\sigma\right]$$

$$\frac{d\langle E \rangle}{dt} = \underbrace{\frac{1}{2}\,\mathrm{Tr}\left[\mathcal{H}(t)\frac{d}{dt}\left(\langle x \rangle\langle x \rangle^T + \sigma\right)\right]}_{\text{Heat}} + \underbrace{\frac{1}{2}\,\mathrm{Tr}\left[\frac{d}{dt}\mathcal{H}(t)\left(\langle x \rangle\langle x \rangle^T + \sigma\right)\right]}_{\text{Work}}$$

Employing the evolution equation for σ and the FD relation, we obtain:

$$\langle \dot{Q} \rangle = \sum_r \underbrace{\left(\langle j_r \rangle\langle v_r \rangle + \mathrm{Tr}[(\mathcal{H}\sigma\mathcal{H} - k_b T_r\mathcal{H})\mathcal{C}_r\mathcal{C}_r^T]\right)}_{\text{Local heat currents?}}$$



Local heat currents are actually given by:

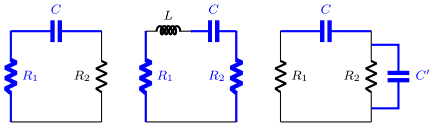
$$\dot{Q}_r = j_r(v_r + \Delta v_r)$$

If there are no fundamental cut-sets simultaneously involving resistors inside and outside the normal tree, then:

$$\langle \dot{Q}_r \rangle = \langle j_r \rangle \langle v_r \rangle + \mathrm{Tr}[(\mathcal{H}\sigma\mathcal{H} - k_b T_r \mathcal{H})\mathcal{C}_r \mathcal{C}_r^T].$$

If not, $\langle \dot{Q}_r \rangle$ is divergent.

Some examples:



(a) (b) (c)

In (a), fluctuations of arbitrarily high frequency in R_2 can be dissipated into R_1.
In (b) and (c) these fluctuations are filtered out.

- This is an artifact of the white noise idealization.
- It indicates that relevant degrees of freedom are not explicitly described.
- This can be solved by taking $S(\omega) = (Rk_b T/\pi)J(\omega)$, with $J(\omega)$ vanishing for large frequencies or, equivalently, by 'dressing' a white noise resistor (analogous to Markovian embedding techniques).

Generalization to quantum noise

Classical Johnson-Nyquist noise: $\langle \Delta v(t) \Delta v(t') \rangle = 2 R k_b T \, \delta(t - t') \implies S(\omega) = \frac{R k_b T}{\pi}$

Quantum Johnshon-Nyquist noise: $\mathcal{S}(\omega) = \frac{R}{\pi} \hbar\omega \, \coth\left(\frac{\hbar\omega}{2k_b T}\right) = \frac{R}{2\pi} \hbar\omega \, (N(\omega) + 1/2)$

Semiclassical treatment:

$$\frac{dx}{dt} = \mathcal{A}(t)\mathcal{H}(t)\, x + \mathcal{B}(t)s(t) + \sum_r \sqrt{2k_b T_r}\, \mathcal{C}_r \, \xi(t) \qquad \mathcal{S}_{\xi_r}(\omega) = \frac{1}{2\pi} \frac{\hbar\omega}{k_b T_r} \, (N_r(\omega) + 1/2)$$

-We do not promote x to quantum operators
-We can directly apply this to overdamped circuits

In this way we obtain:

$$\frac{d}{dt}\sigma(t) = \mathcal{A}\mathcal{H}(t)\sigma(t) + \sigma(t)\mathcal{H}(t)\mathcal{A}^T + \sum_r 2k_b T_r \, \left(\mathcal{I}_r(t)\, \mathcal{C}_r \mathcal{C}_r^T + \mathcal{C}_r \mathcal{C}_r^T \, \mathcal{I}_r(t)^T\right)$$

where:

$$\mathcal{I}_r(t) = \int_0^t d\tau \, G(t, t - \tau) \, \langle \xi_r(0) \xi_r(\tau) \rangle \qquad \frac{d}{dt} G(t, t') - \mathcal{A}(t)\mathcal{H}(t) G(t, t') = \mathbb{1}\delta(t, t')$$

This matches the results of a full quantum treatment for circuits that can be directly quantized (in the Markov approximation)

Generalization of Landauer-Büttiker formula for heat

$$\boxed{\langle \dot{Q}_r \rangle = \langle j_r \rangle \langle v_r \rangle + \sum_{r'} \int_{-\Lambda}^{+\Lambda} d\omega \, \hbar\omega \, f_{r,r'}(t,\omega) \, (N_{r'}(\omega) + 1/2)}$$

Non-diagonal elements: $f_{r,r'}(t,\omega) = \frac{1}{\pi} \mathrm{Tr} \left[\mathcal{H}(t) \hat{G}(t,\omega) \mathcal{D}_{r'} \hat{G}(t,\omega)^\dagger \mathcal{H}(t) \mathcal{D}_r \right] \qquad (r \neq r')$

Sum over first index: $\bar{f}_{r'}(t,\omega) = \sum_r f_{r,r'}(t,\omega) = \frac{1}{2\pi} \mathrm{Tr} \left[\left(\hat{G}^\dagger \frac{d\mathcal{H}}{dt} \hat{G} - \frac{d}{dt} \left(G^\dagger \mathcal{H} \hat{G} \right) \right) \mathcal{D}_{r'} \right]$

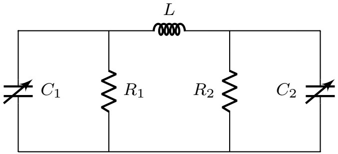
For static circuits ($\bar{f}_{r'} = 0$) we recover the usual Landauer-Büttiker formula

$$\langle \dot{Q}_r \rangle = \langle j_r \rangle \langle v_r \rangle + \sum_{r'} \int_{-\Lambda}^{+\Lambda} d\omega \, \hbar\omega \, f_{r,r'}(\omega) \, (N_{r'}(\omega) - N_r(\omega))$$

General result

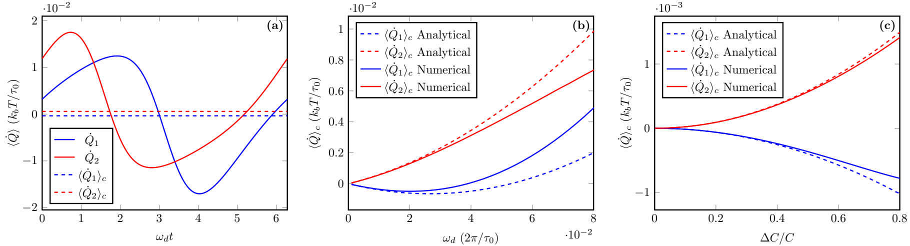
We have derived a generalized Landauer-Büttiker formula which is valid for arbitrary circuits, with any number of resistors at arbitrary temperatures, and for arbitrary driving protocols.

A simple circuit-based machine: cooling a resistor



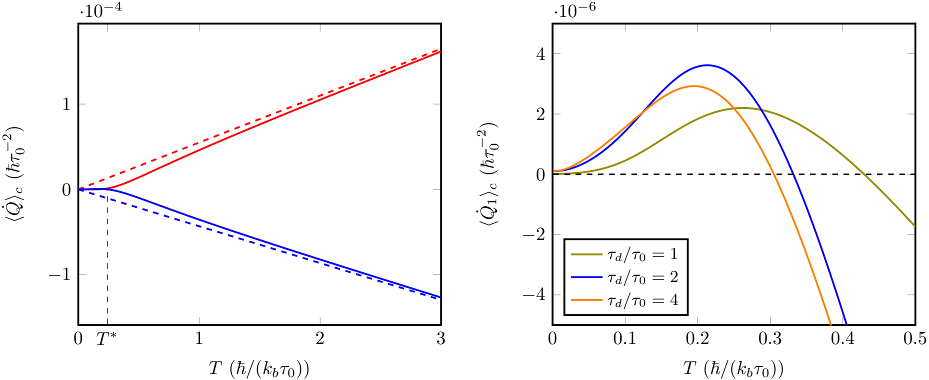
$$C_1 = C + \Delta C \cos(\omega_d t)$$
$$C_2 = C + \Delta C \cos(\omega_d t + \theta)$$

Numerical vs analytical results: (High T, $\tau_0 = \sqrt{LC}$, $\tau_d = RC$, $\tau_0 = \tau_d$)



(a) Asymptotic cycle of the heat currents for $\Delta C/C = 1/2$ and $\omega_d/(2\pi) = 10^{-2}/\tau_d$ (dashed lines indicate cycle averages).
(b) Average heat currents versus driving frequency for $\Delta C/C = 0.5$.
(c) Average heat currents versus driving strength for $\omega_d/(2\pi) = 10^{-2}/\tau_d$.
For all cases we took $\theta = \pi/2$ and $T_1 = T_2 = T$.

Low temperature quantum behaviour:



Conclusions

Stochastic and Quantum Thermodynamics of Driven RLC Networks

Nahuel Freitas,[1] Jean-Charles Delvenne,[1] and Massimiliano Esposito[1]
[1] *Complex Systems and Statistical Mechanics, Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg*

arXiv:1906.11233

Key findings:

- We identified the proper definition of heat under the white noise idealization
- We showed how driven RLC circuits can be used to design thermal machines
- We showed that a semiclassical approach is equivalent to an exact quantum treatment

Ongoing work:

- An analogous (classical) treatment for non-linear devices is under way.