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QUANTUM THERMODYNAMICS:
WHAT IT MEANS AND WHAT IT STRIVES FOR

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Quantum thermodynamics
quantum transport
IFUSP

Grupo Grhafite - IFUSP
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IRREVERSIBILITY

- Consider the simplest possible problem in thermodynamics:
  - A system *S* is put in contact with an environment *E*.
  - As time passes, the state of the system will eventually relax and achieve thermal equilibrium with the bath.

WHAT IS DIFFERENT IN QUANTUM SYSTEMS?

1. THERE ARE OTHER TYPES OF RESOURCES

- In quantum systems there are also other resources, such as *entanglement and coherence*.

- These *Quantum resources* can be used in information processing tasks to obtain *quantum advantages:*

  - Faster algorithms.

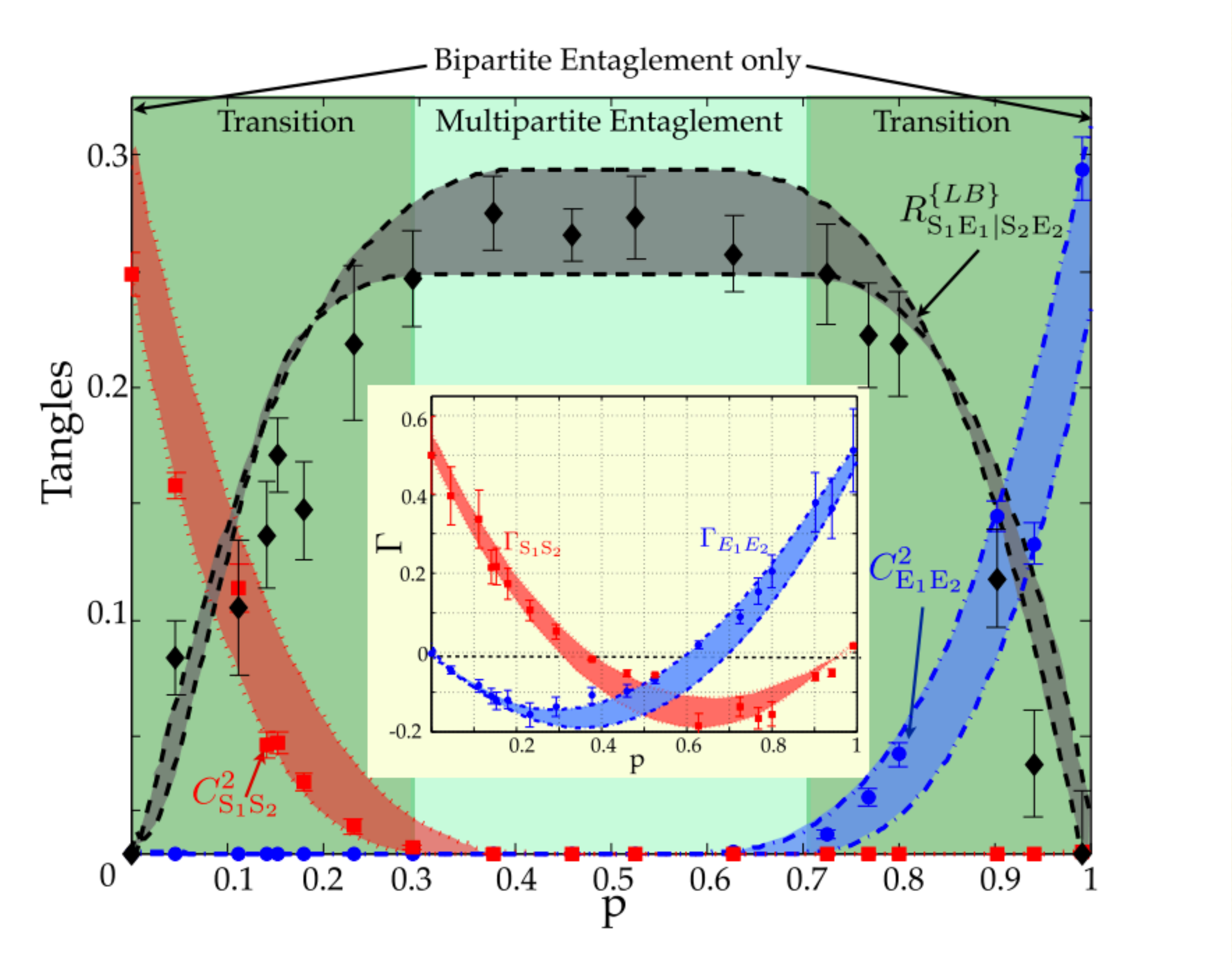
  - More precise measurements (metrology).

  - More secure communications.

  - More efficient quantum simulations.

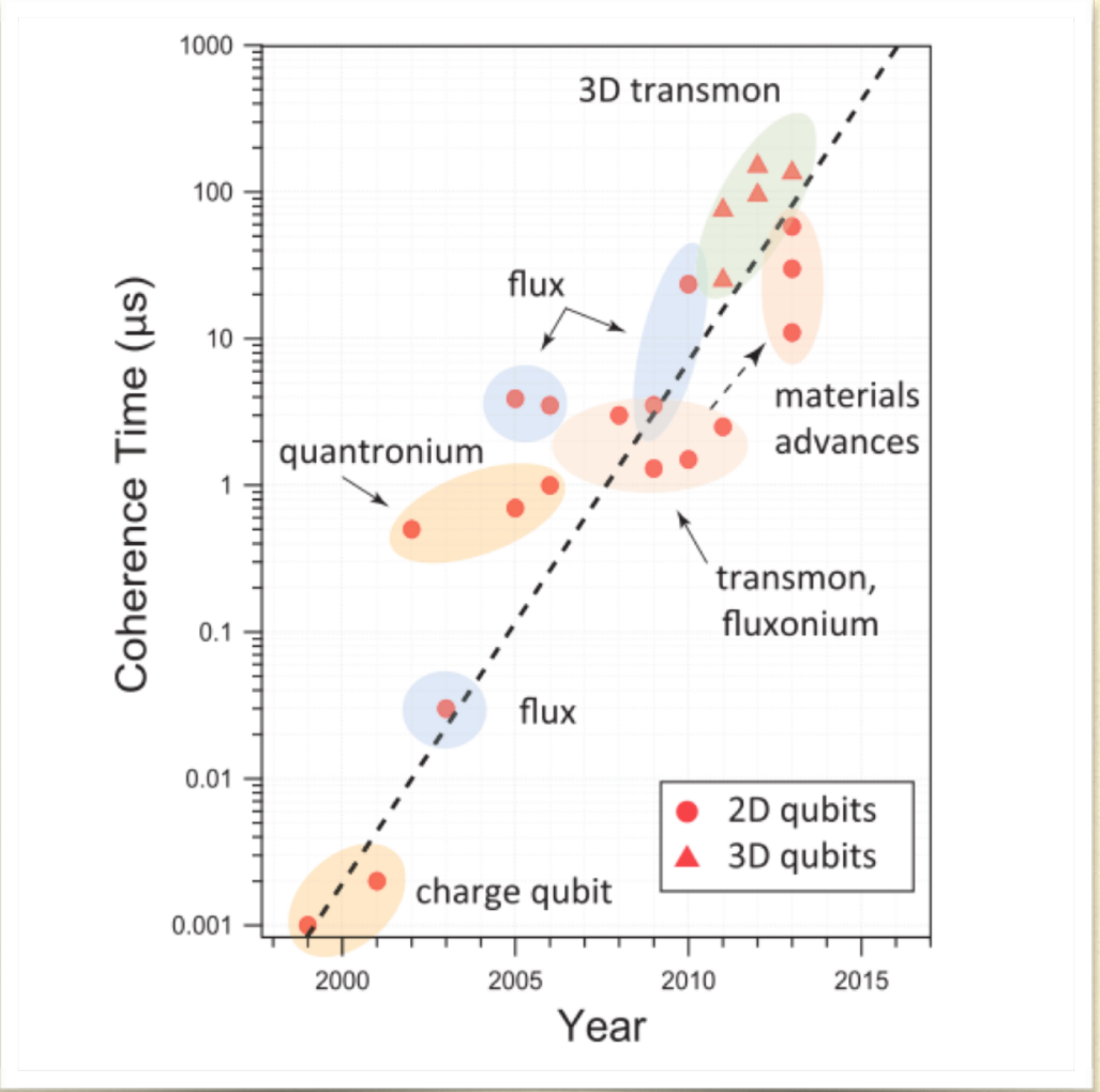
1. THERE ARE OTHER TYPES OF RESOURCES

- But these resources are affected by the contact of with the environment.



Aguilar, Valdés-Hernández, Davidovich, Walborn, Souto Ribeiro, *Phys. Rev. Lett*, **113**, 240501 (2014)

I. THERE ARE OTHER TYPES OF RESOURCES



- **Coherence time.**
- Figure of merit for quantum information processing.
- Amount of time that the system can retain its quantum properties.
- Exponential growth in the last decades in some *platforms*.
- We now have a handful of "*Controlled quantum platforms*".

1. THERE ARE OTHER TYPES OF RESOURCES

- Consider a system of N qubits (i.e. spin 1/2 particles).
- The most general state has the form:

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_N} \psi_{\sigma_1,\ldots,\sigma_N} |\sigma_1,\ldots,\sigma_N\rangle$$

- For instance, a state with an enormous amount of coherence is a *GHZ* state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|1,\ldots,1\rangle + |-1,\ldots,-1\rangle\Big)$$

- This is a superposition of *macroscopically* distinct states. Such a state is a *huge* resource for metrology, for instance.

I. THERE ARE OTHER TYPES OF RESOURCES

- Coherences and entanglement are usually washed away very quickly by the contact of a system with its environment.
- We start with a pure state:

$$|\psi\rangle = a|0\rangle + b|1\rangle \qquad \Longrightarrow \qquad \rho = |\psi\rangle\langle\psi| = \begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix}$$

- Then the contact with the environment will gradually degrade the coherences:

$$\rho(t) = \begin{pmatrix} |a|^2 & e^{-\gamma t} ab^* \\ e^{-\gamma t} a^*b & |b|^2 \end{pmatrix}$$

- If we wait long enough, we eventually get a classical state:

$$\rho(\infty) = \begin{pmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{pmatrix}$$

1. THERE ARE OTHER TYPES OF RESOURCES

- But such a state is also the most sensitive to *decoherence*.
- If we put it in contact with a bath, the density matrix will change as

$$\langle \boldsymbol{\sigma} | \rho | \boldsymbol{\sigma}' \rangle \to \langle \boldsymbol{\sigma} | \rho | \boldsymbol{\sigma}' \rangle e^{\Lambda(\boldsymbol{\sigma}, \boldsymbol{\sigma}')}$$

$$\Lambda(\boldsymbol{\sigma}, \boldsymbol{\sigma}') = -\lambda \sum_i (\sigma_i' - \sigma_i)^2$$

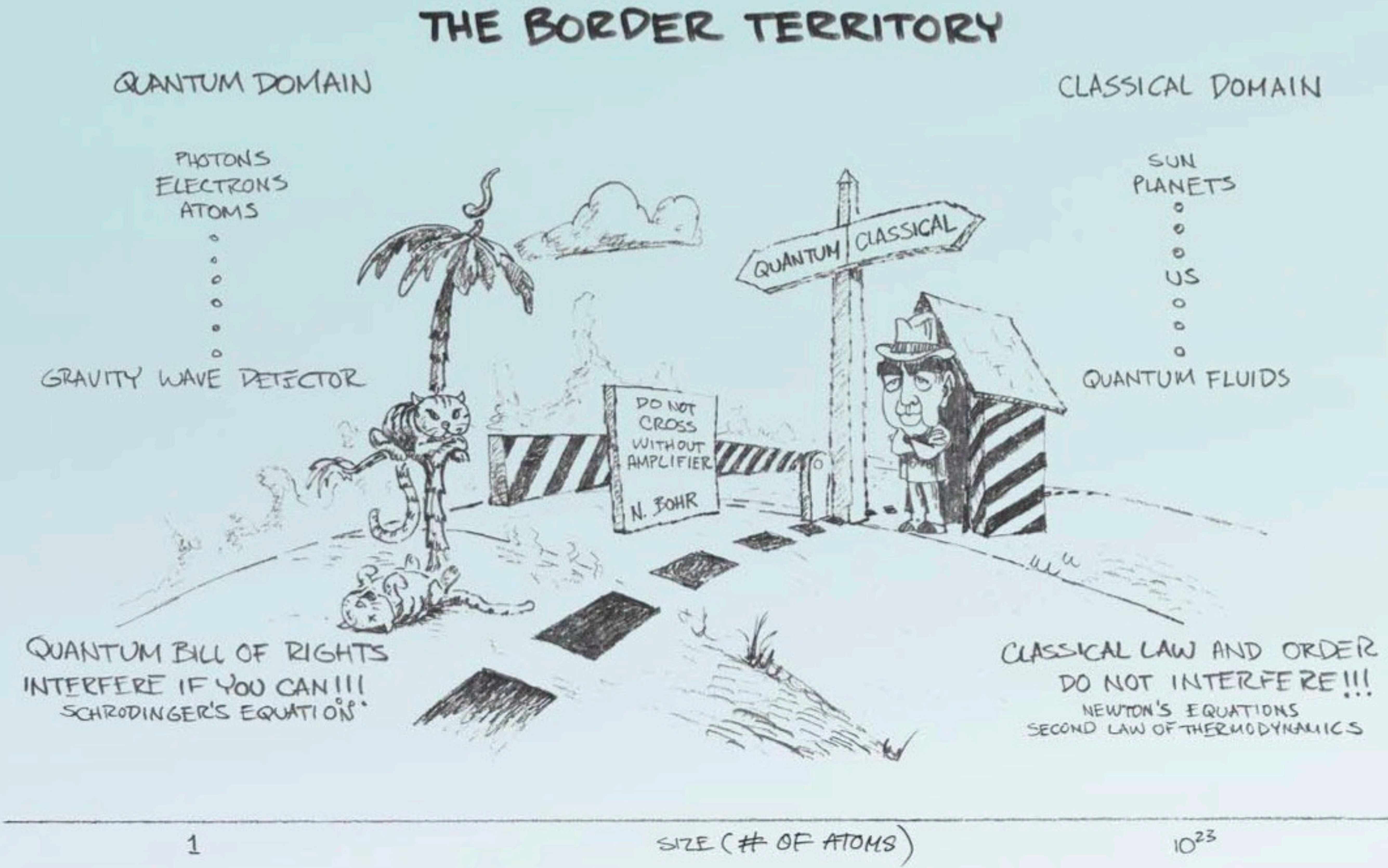
- The decoherence rate is stronger for states which are macroscopically more distinct.

M.A. Cipolla and GTL, *"Processing quantum coherence using the spin-boson model"*, arXiv 1808.01224

2. INFORMATION BECOMES ESSENTIAL

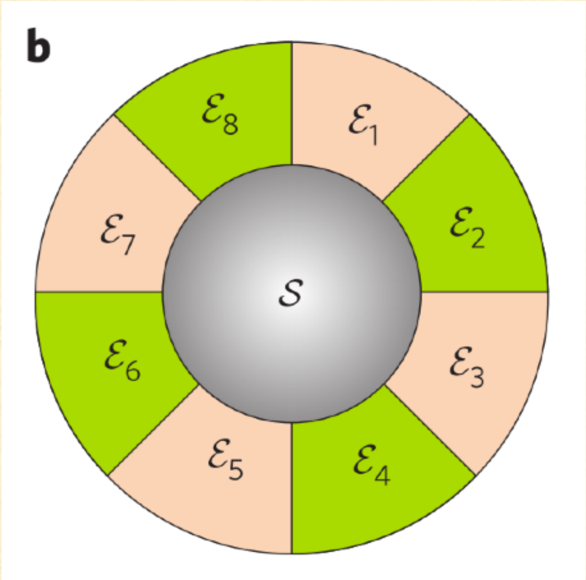
- *"The fragility of states makes quantum systems very difficult to isolate. Transfer of information (which has no effect on classical states) has marked consequences in the quantum realm. So, whereas fundamental problems of classical physics were always solved in isolation (it sufficed to prevent energy loss), this is not so in quantum physics (leaks of information are much harder to plug)."*

W. J. Zurek,
Nature Physics, **5**, 181 (2009)

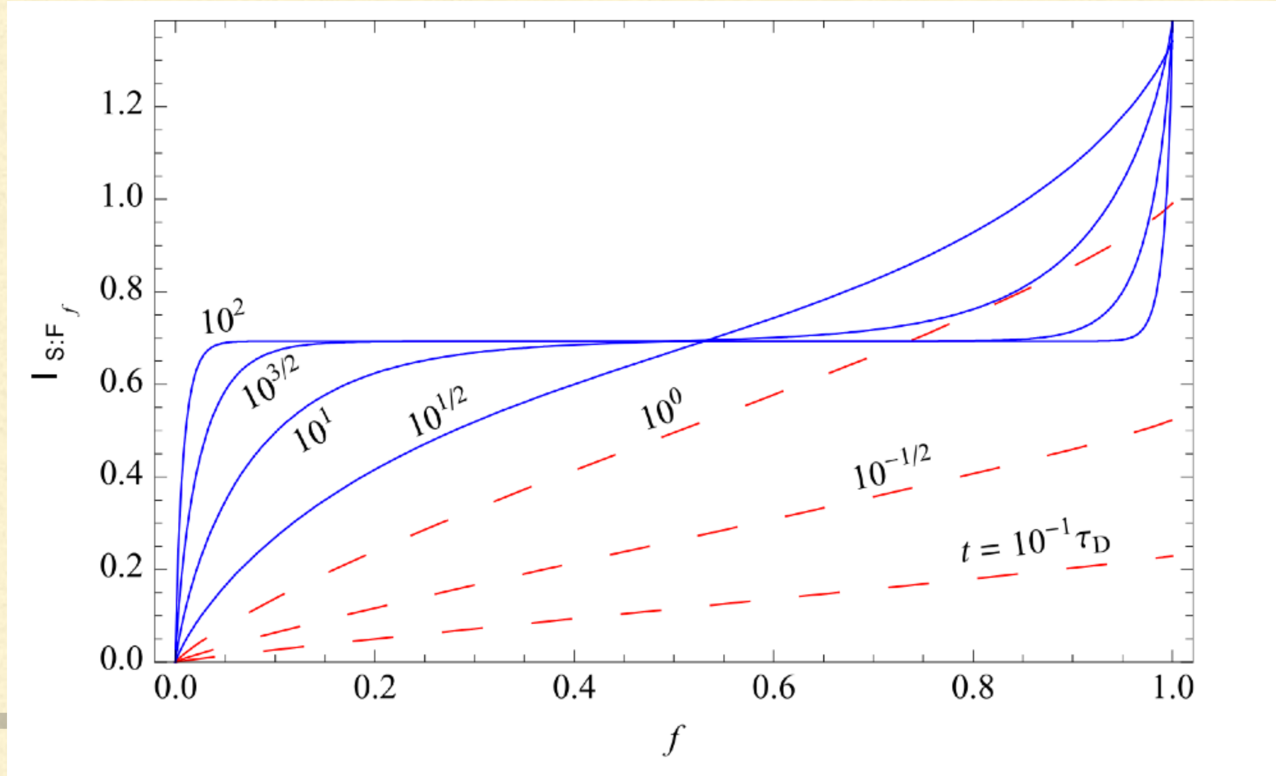

THE BORDER TERRITORY
QUANTUM DOMAIN
CLASSICAL DOMAIN
PHOTONS
ELECTRONS
ATOMS
GRAVITY WAVE DETECTOR
SUN
PLANETS
US
QUANTUM FLUIDS
QUANTUM | CLASSICAL
DO NOT CROSS WITHOUT AMPLIFIER
N. BOHR
QUANTUM BILL OF RIGHTS
INTERFERE IF YOU CAN!!!
SCHRODINGER'S EQUATION
CLASSICAL LAW AND ORDER
DO NOT INTERFERE!!!
NEWTON'S EQUATIONS
SECOND LAW OF THERMODYNAMICS
1
SIZE (# OF ATOMS)
10^23

2. INFORMATION BECOMES ESSENTIAL

- *Objective reality:* why different observers agree on what they are observing.
- The environment in quantum mechanics plays an active role.
- We access the system, by measuring small fractions of the environment.
- e.g.: we measure the fraction of photons scattering from this screen.
  - And we all agree on what we are observing.

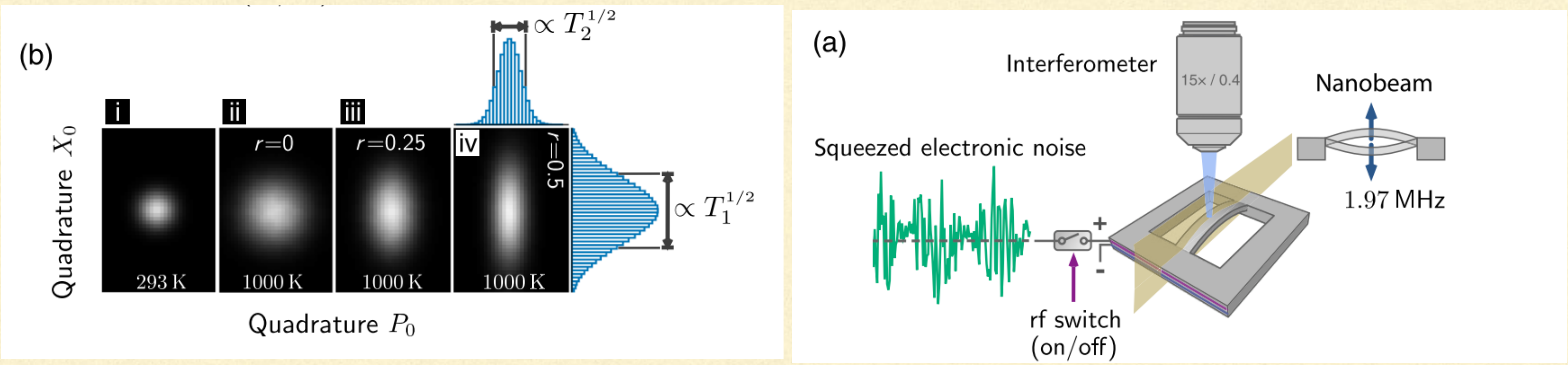


W. J. Zurek,
Nature Physics, **5**, 181 (2009)



3. QUANTUM MECHANICS OFFERS MORE GENERAL BATHS

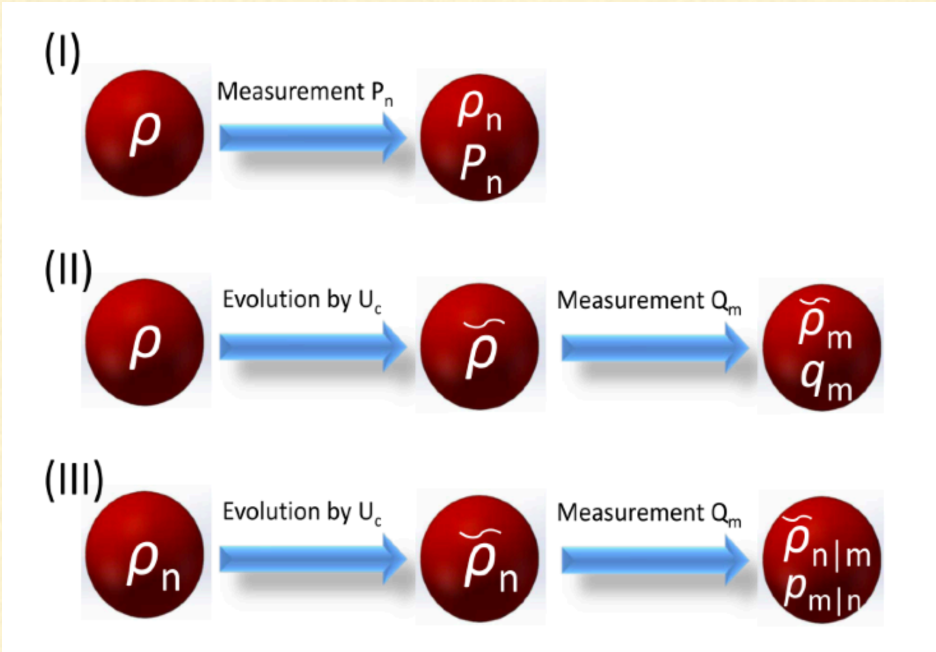
- It is possible to work with *engineered environments*.
- Example: *squeezed thermal bath:*



Klaers, Faelt, Imamoglu, Togan, *Phys. Rev. X*, **7**, 031044 (2017)

Move beyond the standard paradigms of thermodynamics.

4. MEASUREMENTS PLAY A CENTRAL ROLE

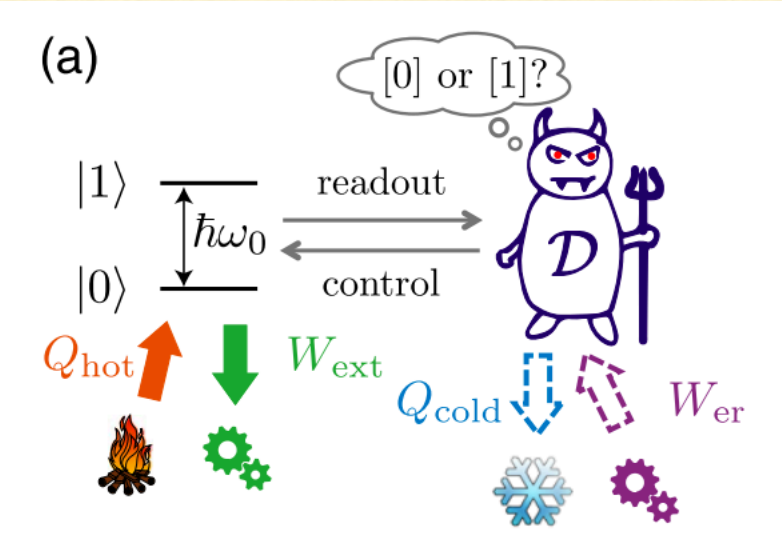


Xiong, *et. al., Phys. Rev. Lett.* **120**, 010601 (2018)

- Back-action (state collapse) affects how we extract thermodynamic information.

- Measurements can be directly implemented in thermodynamic engines.

- Maxwell's demons and information engines.



Elouard, Herrera-Martí, Huard, Auffèves, *Phys. Rev. Lett,* **118**, 260603 (2017)

ENTROPY PRODUCTION

- In thermodynamics the resources are heat and work, and irreversibility is quantified using the *entropy production*.

(Clausius inequality) $$\Delta S \geq \frac{\delta Q}{T} \quad \longrightarrow \quad \Sigma := \Delta S - \frac{\delta Q}{T} \geq 0$$

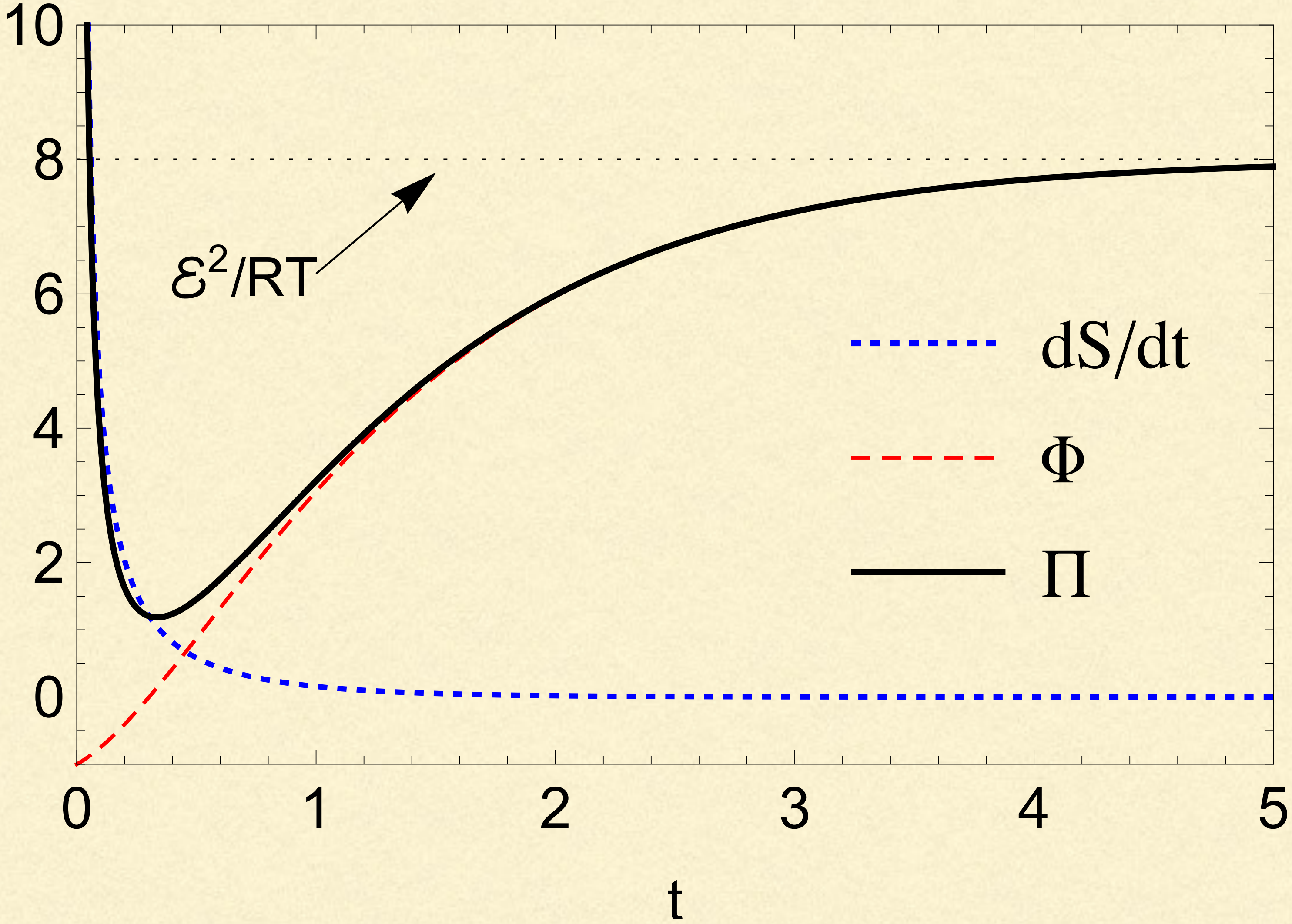
(entropy flux) (entropy production)

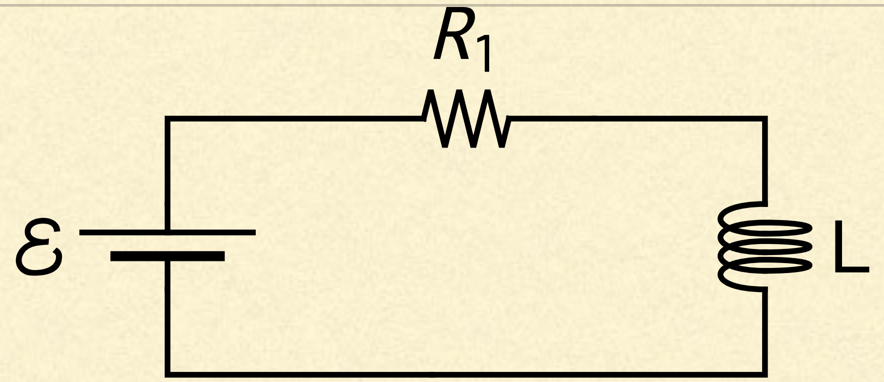
- We also express this in terms of rates:

$$\Pi = \frac{d\Sigma}{dt} \qquad \frac{dS}{dt} = \Pi - \Phi \qquad \Phi = -\frac{1}{T}\frac{dQ}{dt}$$

(entropy production *rate*) (entropy flux *rate*)

EXAMPLE: RL CIRCUIT



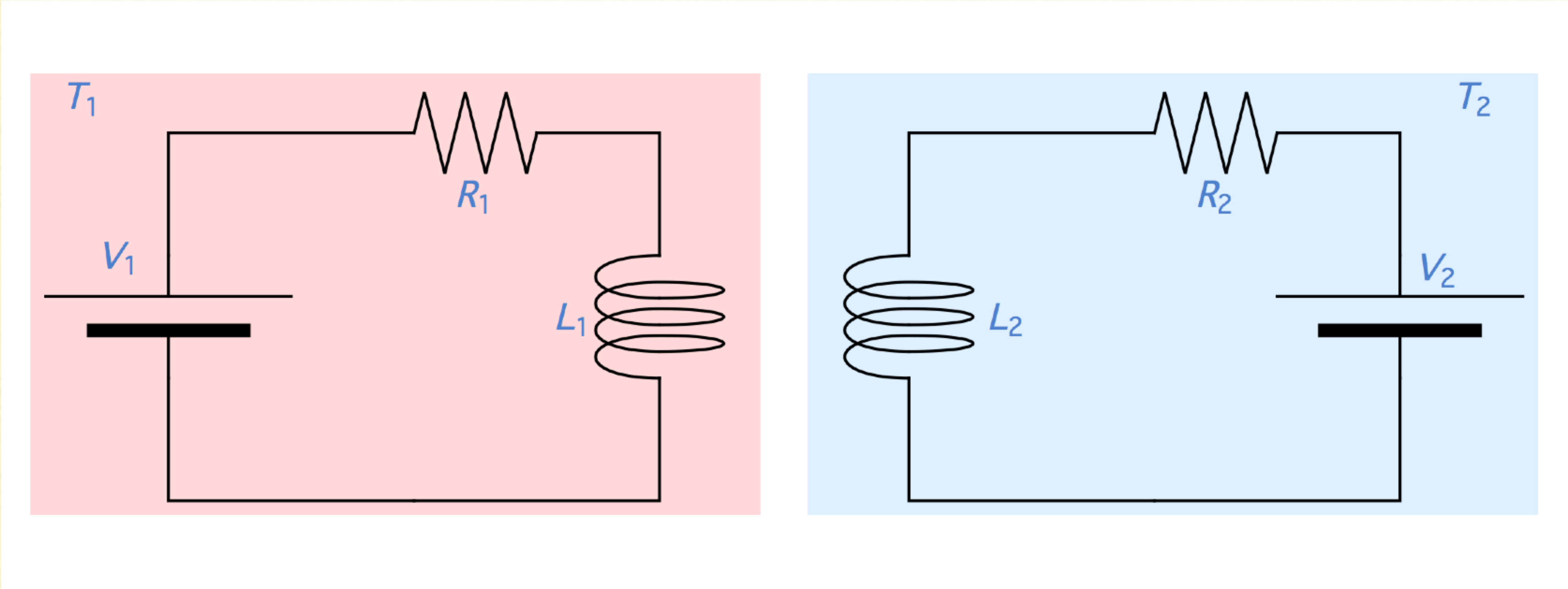


Steady-state

$$\frac{dS}{dt} = 0$$

$$\Pi_{\mathrm{ss}} = \Phi_{\mathrm{ss}} = \frac{\mathcal{E}^2}{RT}$$

EXAMPLE: TWO INDUCTIVELY COUPLED RL CIRCUITS



$$\Pi_{ss} = \frac{\mathcal{E}_1^2}{R_1 T_1} + \frac{\mathcal{E}_2^2}{R_2 T_2} + \frac{m^2 R_1 R_2}{(L_1 L_2 - m^2)(L_2 R_1 + L_1 R_2)} \frac{(T_1 - T_2)^2}{T_1 T_2}$$

GTL, T. Tomé and M. J. de Oliveira, *J. Phys A.* **46** (2013) 395001

CLASSICAL VS. QUANTUM MASTER EQUATIONS

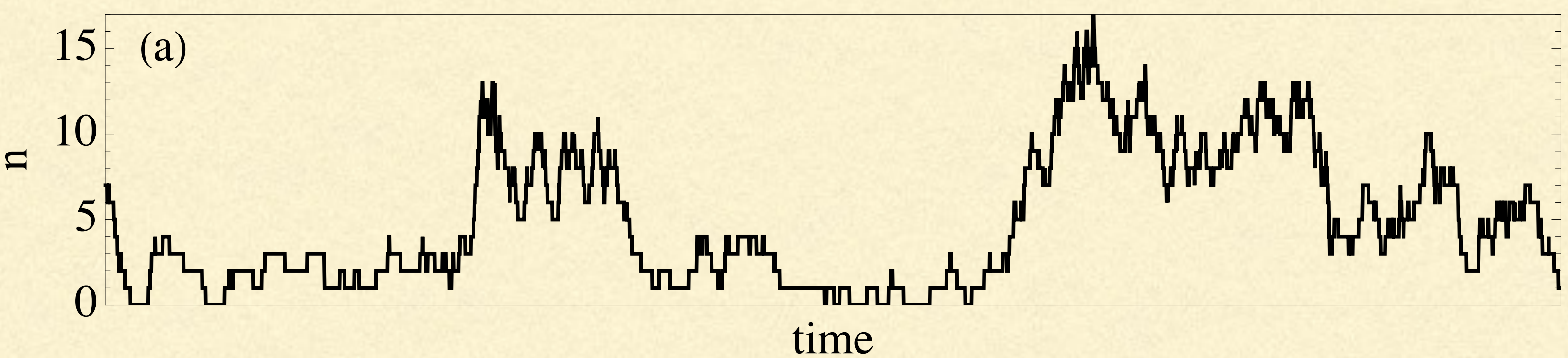
Jader P. Santos, Lucas C. Céleri, Gabriel T. Landi and Mauro Paternostro
The role of quantum coherence in non-equilibrium entropy production
arXiv 1707.08946 (submitted to *Nature Quantum Information*)

- Consider a system with discrete energy levels and let p_n denote de probability of being found in state *n*.

- In a classical approach, the dynamics of the system in contact with a bath would be described by a Pauli master equation:

$$\frac{dp_n}{dt} = \sum_m \left\{ K(n|m)p_m - K(m|n)p_n \right\}$$

- Contact with the bath generates a stochastic motion.



- Microscopically, the system will keep on jumping around, with an average probability given by the equilibrium distribution:

$$p_n^{\mathrm{eq}} = \frac{e^{-\beta E_n}}{Z}$$

- Schnakenberg [Rev. Mod. Phys., **48**, 571 (1976)] found:

$$\Pi = \frac{1}{2}\sum_{n,m}\left\{K(n|m)p_m - K(m|n)p_n\right\}\ln\frac{K(n|m)p_m}{K(m|n)p_n}$$

$$\Phi = \sum_{n,m} K(m|n)p_n \ln\frac{K(m|n)}{K(n|m)}$$

- Thermal states satisfy detailed balance:

$$\frac{K(n|m)}{K(m|n)} = \frac{p_n^{\text{eq}}}{p_m^{\text{eq}}} = e^{-\beta(E_n - E_m)}$$

- So that in this case we recover the thermal scenario:

$$\Phi = \frac{\dot{Q}}{T}$$

See T. Tomé and M. J. de Oliveira, *Dinâmica Estocástica*, EDUSP.

- The entropy production may be written in a cooler way as

$$\Pi = -\frac{dS(\mathbf{p}(t)||\mathbf{p}^{\mathrm{eq}})}{dt}$$

- Where

$$S(\mathbf{p}||\mathbf{p}^{\mathrm{eq}}) = \sum_n p_n \ln p_n / p_n^{\mathrm{eq}}$$

- is the *Relative entropy* or *Kullback-Leibler divergence.*
- It gives a type of "distance" between probability distributions.

Π due to system adapting to new population imposed by the bath.

OPEN QUANTUM SYSTEMS

- When we first learn quantum mechanics, we introduce *untiaries* as the operators which take kets to kets, preserving probability.

$$|\psi'\rangle = U|\psi\rangle, \qquad U^\dagger U = 1$$

- But then we learn about density matrices.

- We should then redo the question: *what is the most general type of operation which takes density matrices into density matrices?*

- Answer: **a quantum operation:**

$$\rho' = \sum_k M_k \rho M_k^\dagger, \qquad \sum_k M_k^\dagger M_k = 1$$

LINDBLAD MASTER EQUATIONS

- The quantum operation is a *map* (like the unitary).
- If we want a differential equation to *generate* the map, we get instead Lindblad's equation:

$$\frac{d\rho}{dt} = -i[H,\rho] + \sum_k \gamma_k \left[L_k \rho L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho\} \right]$$

- The L's are *jump operators:* they describe how the environment induces jumps in the system.

EXAMPLE: QUBIT

$$\frac{d\rho}{dt} = -i[H,\rho] + D(\rho)$$

$$D(\rho) = \gamma(1-f)\left[\sigma_-\rho\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-,\rho\}\right] + \gamma f\left[\sigma_+\rho\sigma_- - \frac{1}{2}\{\sigma_-\sigma_+,\rho\}\right]$$

$$f = \frac{1}{e^{\beta\Omega}+1}$$

$$\rho = \begin{pmatrix} p_0 & q \\ q^* & p_1 \end{pmatrix}$$

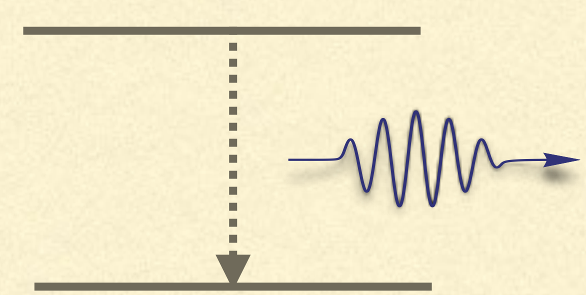
$$\frac{dp_0}{dt} = \gamma f p_1 - \gamma(1-f)p_0$$

$$\frac{dp_1}{dt} = \gamma(1-f)p_0 - \gamma f p_1$$

(Pauli master equation)

$$\frac{dq}{dt} = -\frac{\gamma}{2}q$$

(Decoherence)



ENTROPY PRODUCTION

- Here we consider **Thermal Operations** (or Davies maps), which have simple thermal properties.
  - Thermalize correctly.
  - Populations evolve according to classical M Eq.
- The entropy flux does not depend on the coherences: $$\Phi = -\frac{1}{T}\frac{dQ}{dt}$$
- But the entropy production, on the other hand, becomes.

$$\Pi = -\frac{dS(\rho||\rho_{\rm eq})}{dt}$$

$$S(\rho||\rho_{\rm eq}) = \mathrm{tr}\Big\{\rho(\ln\rho - \ln\rho_{\rm eq})\Big\}$$

GLOBAL UNITARY DYNAMICS

- We can instead think about entropy production in terms of the *global* unitary dynamics of S+E. Then one may show that

$$\Pi = -\frac{d\mathcal{I}_{SE}}{dt} + \frac{dS(\rho_E(t)||\rho_E^{\text{th}})}{dt}$$

- Thus, entropy production stems from:

1. *Mutual information* built up between S and E that is lost.

$$\mathcal{I}_{SE} = S(\rho_S) + S(\rho_E) - S(\rho_{SE})$$

2. The state of the environment being pushed away from equilibrium.

1707.08946 and 1804.02970
see also: M. Esposito, K. Lindenberg, and C. Van Den Broeck, NJP **12**, 013013 (2010).

CONTRIBUTION FROM COHERENCES

- But now we can separate:

$$S(\rho||\rho_{\text{eq}}) = S(\mathbf{p}||\mathbf{p}^{\text{eq}}) + \mathcal{C}(\rho)$$

$$\mathcal{C}(\rho) = S(\Delta_H(\rho)) - S(\rho)$$ (Entropy of coherence)

- As a result, we find that the entropy production can be divided in two parts:

$$\Pi = -\frac{dS(\mathbf{p}(t)||\mathbf{p}^{\text{eq}})}{dt} - \frac{\mathcal{C}(\rho)}{dt}$$

- One part is the classical: entropy production due to population change.
- But the other is genuinely quantum mechanical:
  - Entropy production due to loss of coherence.

QUANTUM PHASE SPACE FORMULATION

Jader P. Santos, Gabriel T. Landi and Mauro Paternostro
The Wigner entropy production rate
Phys. Rev. Lett, **118**, 220601 (2017)

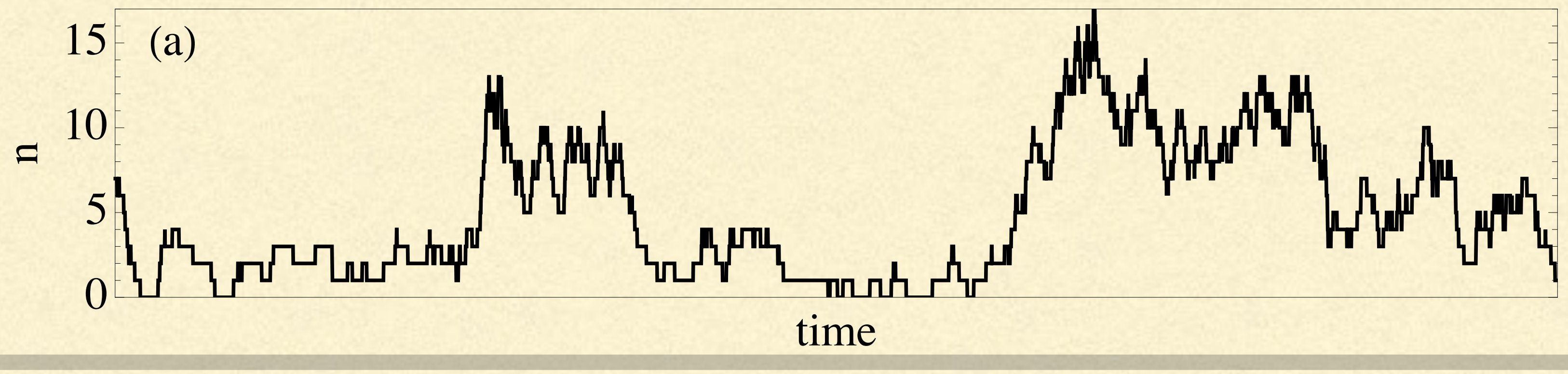
- We shall consider the relaxation of a bosonic mode in contact with a bath:

$$\frac{d\rho}{dt} = -i[H, \rho] + D(\rho)$$

$$H = \omega(a^\dagger a + 1/2)$$

$$D(\rho) = \gamma(\bar{n}+1)\left[a\rho a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\}\right] + \gamma\bar{n}\left[a^\dagger \rho a - \frac{1}{2}\{a a^\dagger, \rho\}\right]$$

$$\bar{n} = \frac{1}{e^{\beta\omega} - 1}$$

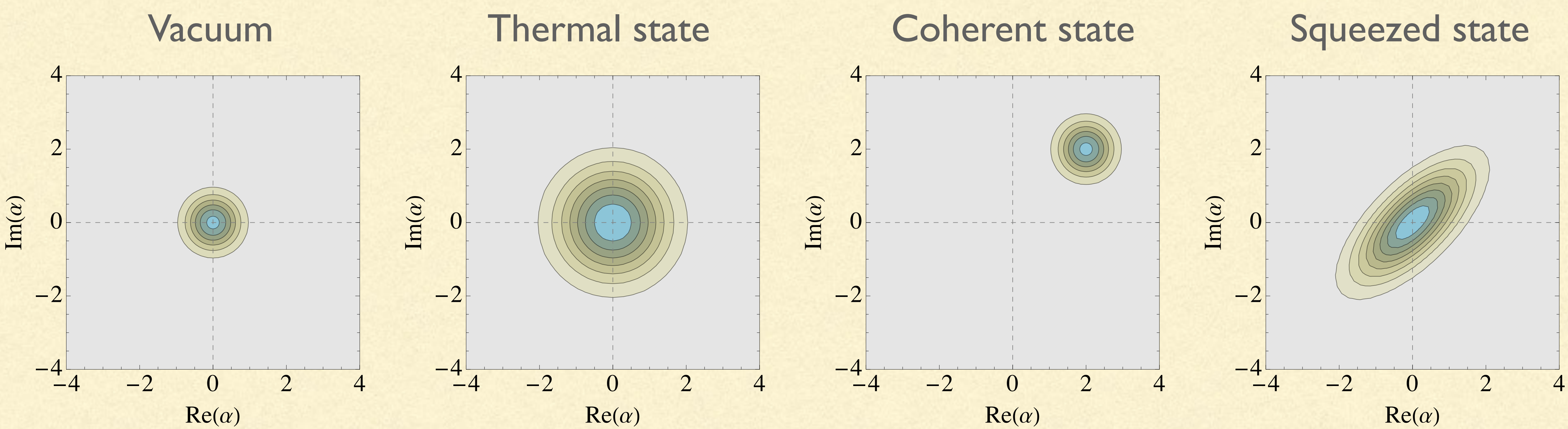


- Instead of working with density matrices, we work with the **Wigner function:**

$$W(\alpha,\alpha^*) = \frac{1}{\pi^2}\int d^2\lambda e^{\lambda^*\alpha-\lambda\alpha^*}\mathrm{tr}\left\{\rho e^{\lambda a^\dagger-\lambda^* a}\right\}$$

$$\mathrm{Re}(\alpha) = q$$
$$\mathrm{Im}(\alpha) = p$$

Introduces the notion of quantum phase space



- The Wigner function will satisfy a *Quantum Fokker-Planck equation*

$$\partial_t W = \partial_\alpha J(W) + \partial_\alpha^* J^*(W)$$

$$J(W) = \frac{\gamma}{2}\Big[\alpha W + (\bar{n} + 1/2)\partial_{\alpha^*} W\Big]$$

- This is a *continuity equation* for the quasi-probability.
- J(W) is a probability current.
- The current is zero if and only if the system is in thermal equilibrium.

$$J(W_{\rm eq}) = 0 \qquad\qquad W_{\rm eq}(\alpha, \alpha^*) = \frac{1}{\pi(\bar{n} + 1/2)} e^{-\frac{|\alpha|^2}{\bar{n}+1/2}}$$

WIGNER ENTROPY

- Instead of using the von Neumann entropy, we adopt instead the entropy of the Wigner function:

$$S = -\int d^2\alpha \; W \ln W$$

- This will be real for Gaussian states (because then W > 0).

- Moreover, it coincides with the Rényi-2 entropy

$$S_2 = -\ln \mathrm{tr}\rho^2$$

Adesso, Girolami, Serafini, *PRL*, **109**, 190502 (2012)

- With the Wigner entropy we can now separate

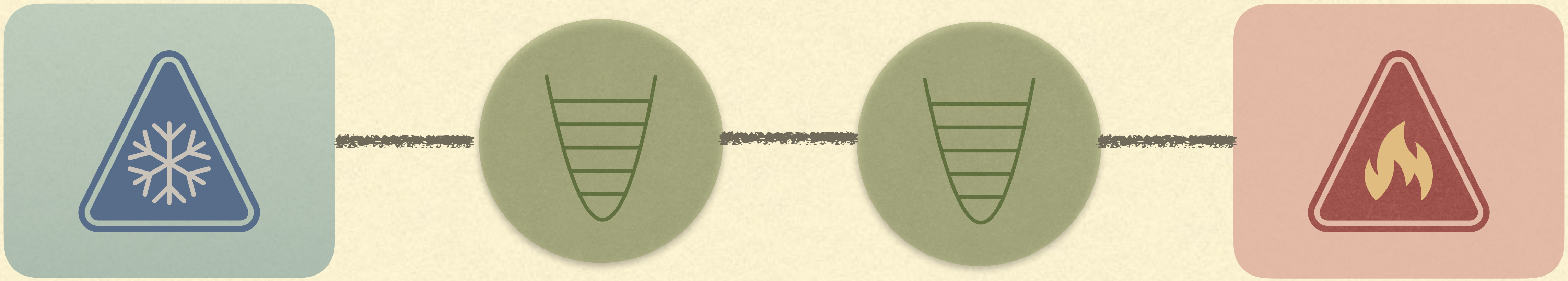
$$\frac{dS}{dt} = \Pi - \Phi$$

- As a result, we find

$$\Pi = \frac{4}{\gamma(n+1/2)} \int d^2\alpha \, \frac{|J(W)|^2}{W} = -\frac{dS(W||W_{\text{eq}})}{dt}$$

$$\Phi = \frac{\gamma}{n+1/2}\Big[\langle a^\dagger a\rangle - n\Big] = -\frac{1}{\omega(n+1/2)}\frac{dQ}{dt}$$

- At high temperatures $\omega(n+1/2) \simeq T$ which leads to $\Phi \simeq -\frac{1}{T}\frac{dQ}{dt}$

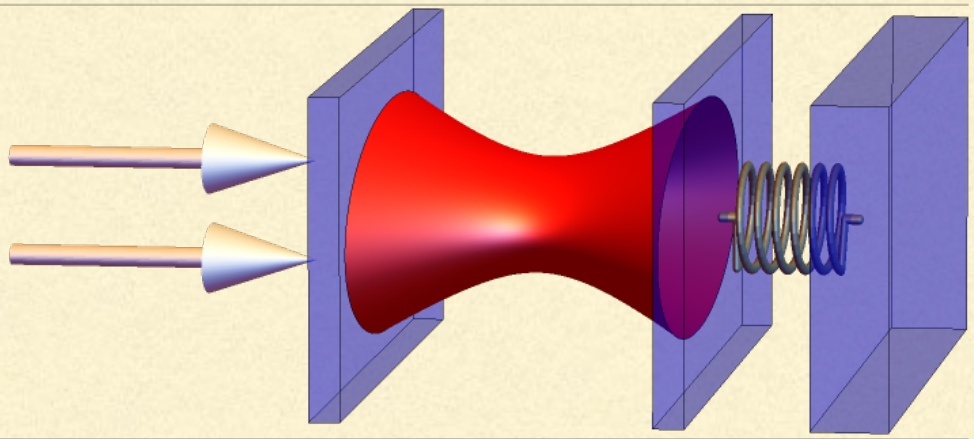


NON-EQUILIBRIUM STEADY-STATES (NESS)

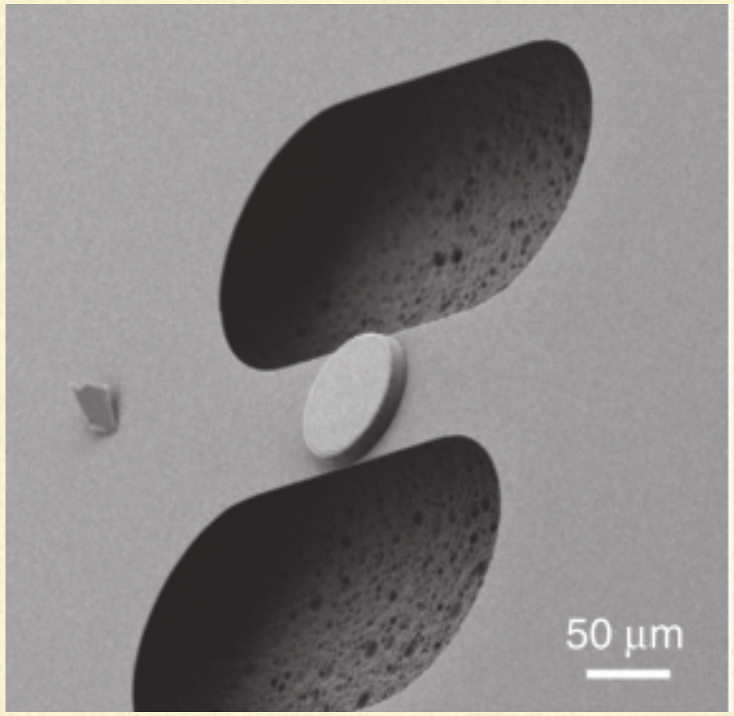
William B. Malouf, Jader P. Santos, Mauro Paternostro and Gabriel T. Landi
Wigner entropy production in quantum non-equilibrium steady-states
In preparation *(2018).*

M. Brunelli, *et. al.,* arXiv 1602.06958. Accepted in PRL.

OPTOMECHANICS



- A thin membrane is allowed to vibrate in contact with radiation trapped in a cavity.



Aspelmeyer group
Viena

$$H = \omega_c a^\dagger a + \left(\frac{p^2}{2m} + \frac{1}{2} m \omega_m^2 x^2 \right)$$

$$-g a^\dagger a x + \epsilon (a^\dagger e^{-i\omega_p t} + a e^{i\omega_p t})$$

$$\frac{d\rho}{dt} = -i[H, \rho] + D_c(\rho) + D_m(\rho)$$

Groeblacher, *et. al.*, Nature Communications, **6**, 7606 (2015)

$$\frac{d\rho}{dt} = -i[H,\rho] + D_c(\rho) + D_m(\rho)$$

- The system tends to a NESS because there are two dissipation channels.
- The mechanical oscillator has the usual damping:

$$D_m(\rho) = \gamma(n_m+1)\left[b\rho b^\dagger - \frac{1}{2}\{b^\dagger b,\rho\}\right] + \gamma n_m \left[b^\dagger \rho b - \frac{1}{2}\{bb^\dagger,\rho\}\right]$$

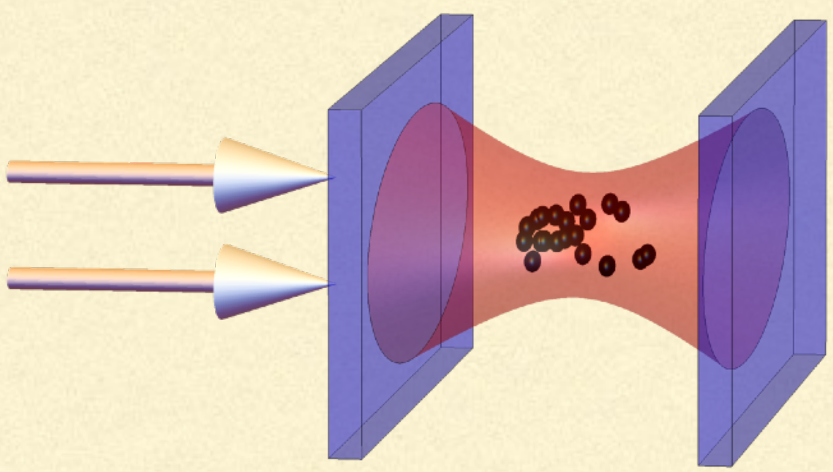
- where γ is the coupling rate to the environment and $n_m = \frac{1}{e^{\omega_m/T}-1}$
- On the other hand, the cavity can also loose photons (this is how they measure the cavity), which is described by

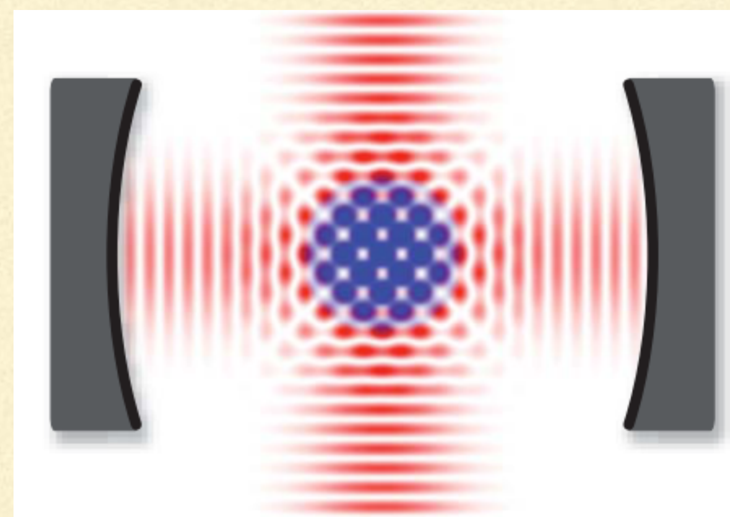
$$D_c(\rho) = 2\kappa\left[a\rho a^\dagger - \frac{1}{2}\{a^\dagger a,\rho\}\right]$$

DRIVEN-DISSIPATIVE BEC

Esslinger group
ETH

- Another interesting quantum NESS is that of a BEC interacting with a cavity field.





b_0 and b_1 are bosonic operators of the ground-state and first excited state of the BEC

$$H = \omega_c a^\dagger a + \frac{\omega_0}{2}(b_1^\dagger b_1 - b_0^\dagger b_0) + \frac{2\lambda}{\sqrt{N}}(a + a^\dagger)(b_0^\dagger b_1 + b_1^\dagger b_0)$$

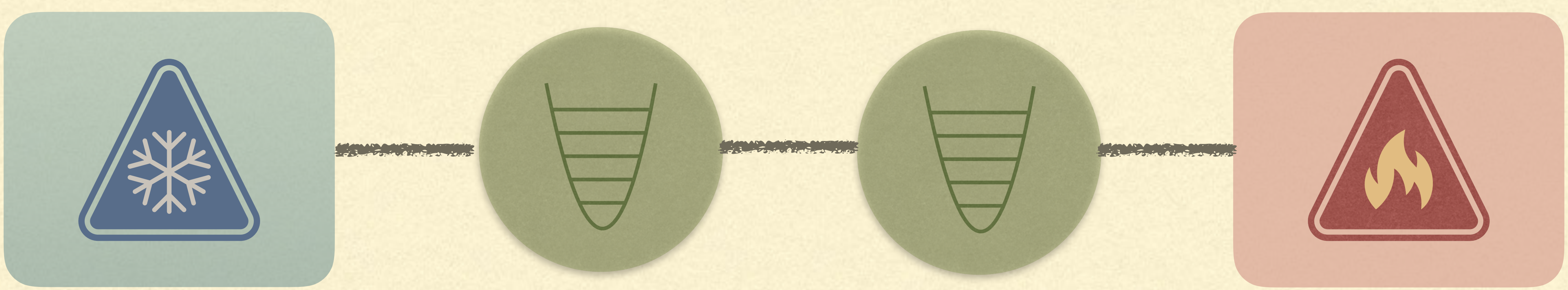
Baumann, *et. al.*,Nature, **464**,1301 (2010)

GAUSSIANIZATION

- Both models can be Gaussianized for large drive and converted into an effective system of two harmonic oscillators

$$H = \omega_a a^\dagger a + \omega_b b^\dagger b + g(a + a^\dagger)(b + b^\dagger)$$

- For the BEC, the mode *b* is a collective (Schwinger) mode of the atomic system.

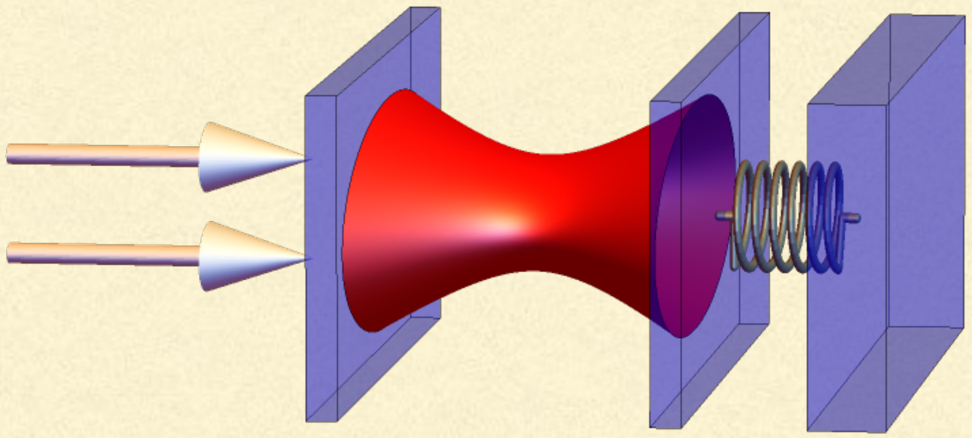


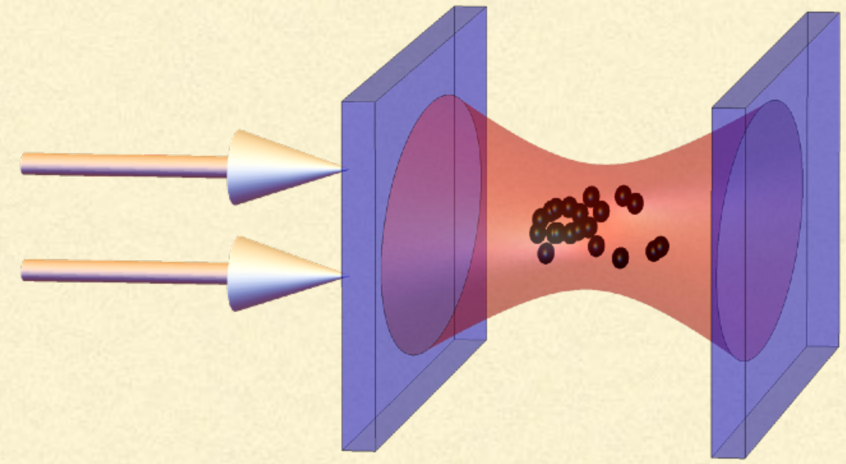
TROUBLE @T = 0

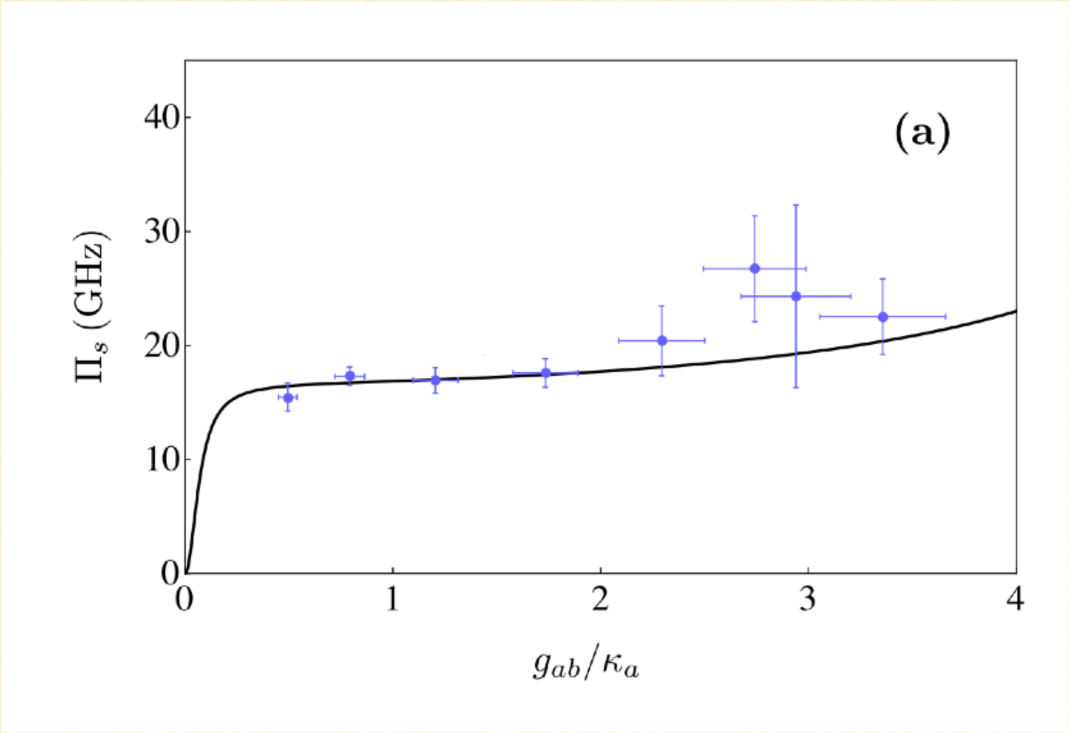
$$D_c(\rho) = 2\kappa\left[a\rho a^\dagger - \frac{1}{2}\{a^\dagger a, \rho\}\right]$$

- Both models clearly correspond tend to a quantum NESS.
- However, in both cases one of the reservoirs is the photon loss bath.
  - which behaves exactly as a thermal bath at zero temperature.
- The von Neumann description of breaks down at T = 0.
  - Both production and flux diverge.
- The Wigner framework is therefore *the* only framework capable of describing entropy production in these systems.

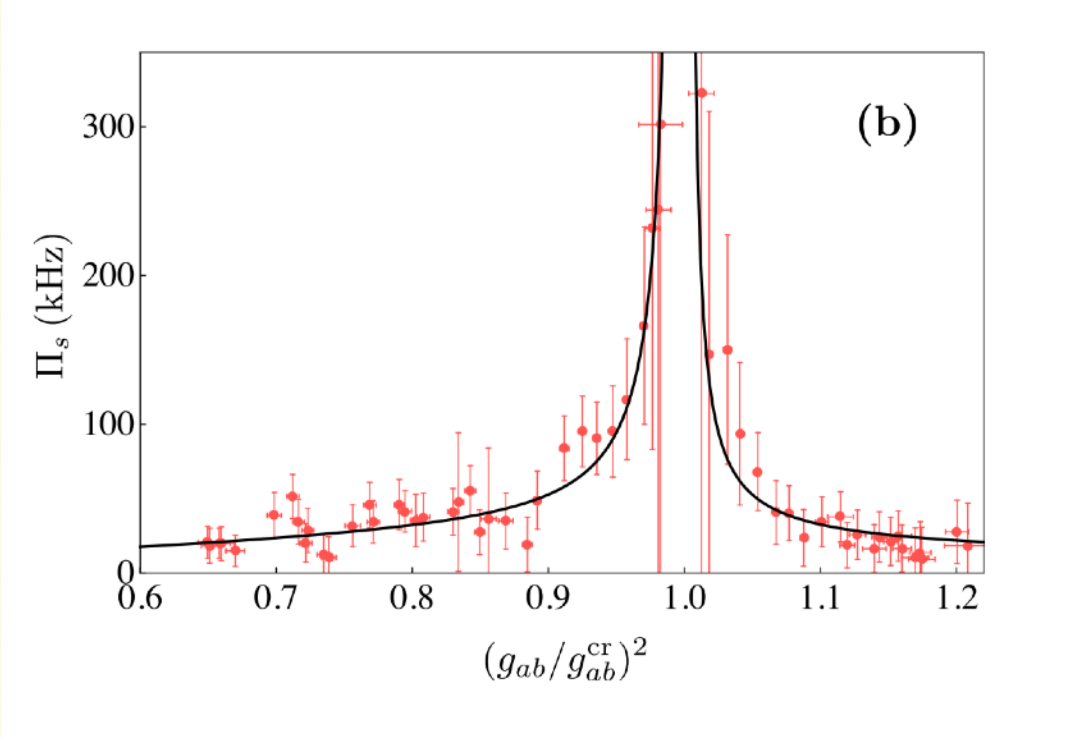
RESULTS







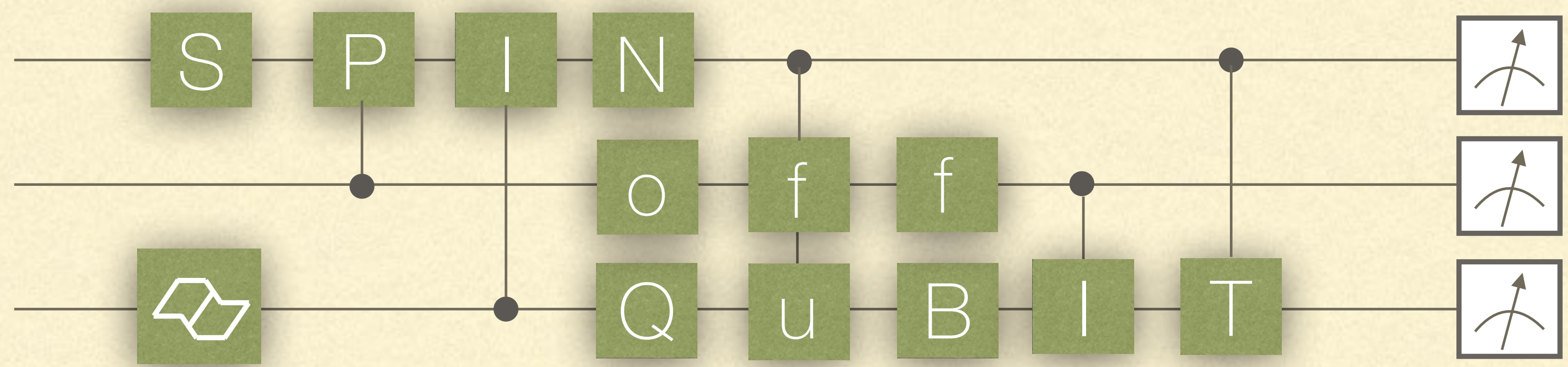
optomechanics



BEC

CONCLUSIONS

- Thermodynamics at the quantum level mixes classical and quantum resources.
  - Important as a tool for applications in quantum information processing.
- But the theory is far from complete. Exciting field, with new developments happening all the time.
- Highly interdisciplinary, with connections to condensed matter, quantum gases, high-energy physics and etc.



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Thanks.

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