33rd Chris Engelbrecht Summer School

April 2025

Introduction to Quantum Thermodynamics

Lecture 1

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Lecture I: Thermodynamic framework in the quantum regime

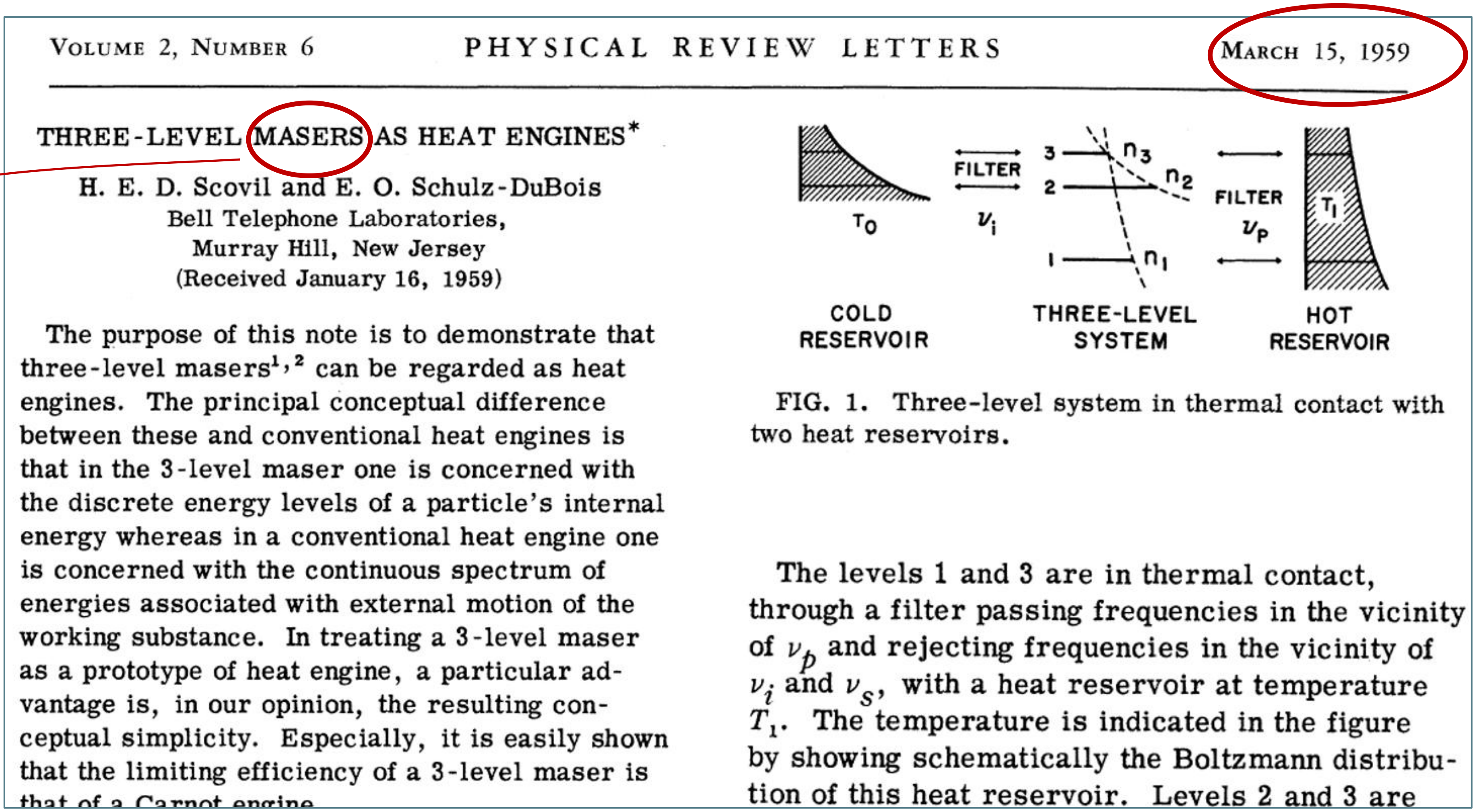
I. Brief historical perspective
II. Current problematics of Quantum Thermodynamics
III. Work and Heat
  – Classical systems
  – Extension to stochastic classical thermodynamics
  – Standard definitions of work and heat for quantum systems.
  – Some limitations
IV. Opening: brief overview of current state of the research

I. Brief historical perspective

Brief historical perspective:

- First research articles on what will become Quantum Thermodynamics appeared from the years 1960 to 1980.

→ Papers mainly discussing the extension of thermal machines and Carnot cycle to quantum systems:



Volume 2, Number 6 PHYSICAL REVIEW LETTERS March 15, 1959

THREE-LEVEL MASERS AS HEAT ENGINES*

H. E. D. Scovil and E. O. Schulz-DuBois
Bell Telephone Laboratories,
Murray Hill, New Jersey

(Received January 16, 1959)

The purpose of this note is to demonstrate that three-level masers[1,2] can be regarded as heat engines. The principal conceptual difference between these and conventional heat engines is that in the 3-level maser one is concerned with the discrete energy levels of a particle's internal energy whereas in a conventional heat engine one is concerned with the continuous spectrum of energies associated with external motion of the working substance. In treating a 3-level maser as a prototype of heat engine, a particular advantage is, in our opinion, the resulting conceptual simplicity. Especially, it is easily shown that the limiting efficiency of a 3-level maser is that of a Carnot engine

FIG. 1. Three-level system in thermal contact with two heat reservoirs.

The levels 1 and 3 are in thermal contact, through a filter passing frequencies in the vicinity of ν_p and rejecting frequencies in the vicinity of ν_i and ν_s, with a heat reservoir at temperature T_1. The temperature is indicated in the figure by showing schematically the Boltzmann distribution of this heat reservoir. Levels 2 and 3 are

“Laser” but elecromagnetic in the range of the microwave (wavelength between 1mm and 1m)

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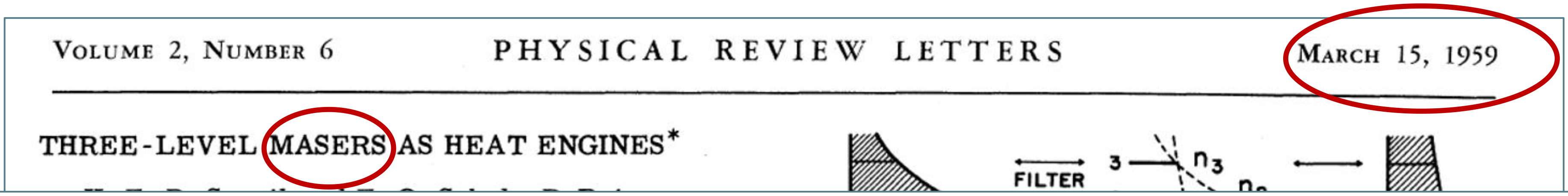

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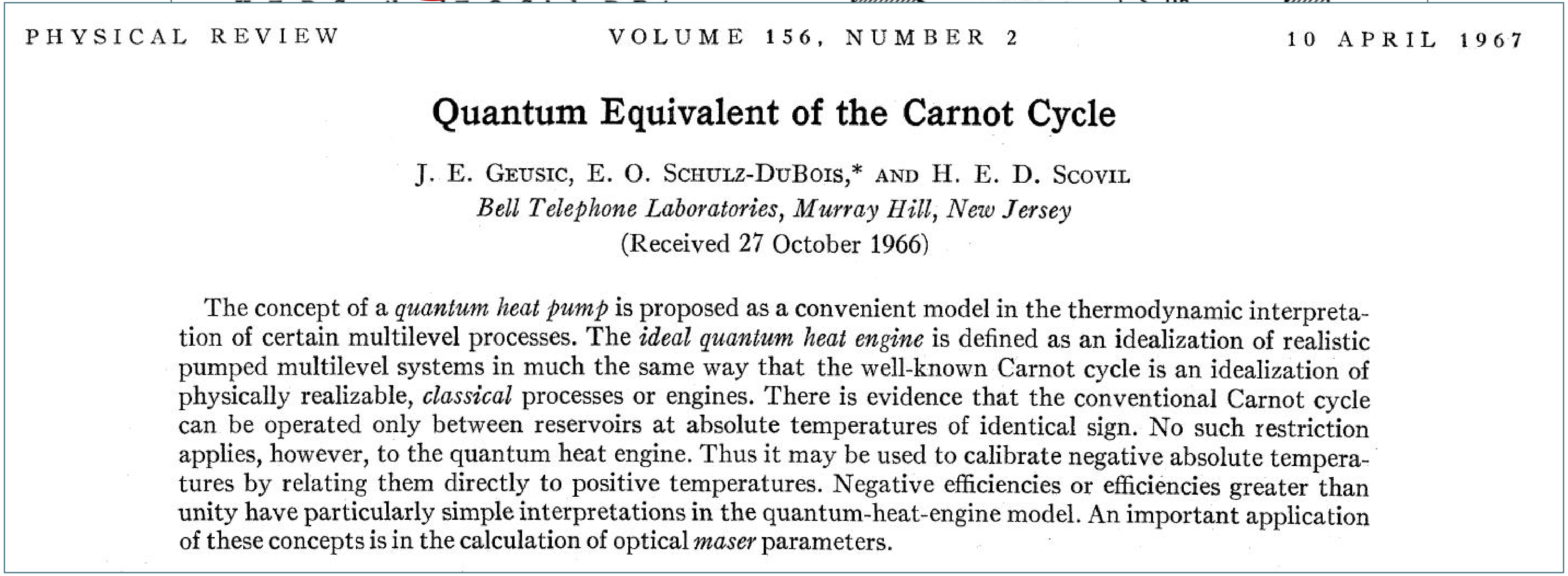

PHYSICAL REVIEW VOLUME 156, NUMBER 2 10 APRIL 1967

Quantum Equivalent of the Carnot Cycle

J. E. GEUSIC, E. O. SCHULZ-DUBOIS,* AND H. E. D. SCOVIL
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received 27 October 1966)

The concept of a *quantum heat pump* is proposed as a convenient model in the thermodynamic interpretation of certain multilevel processes. The *ideal quantum heat engine* is defined as an idealization of realistic pumped multilevel systems in much the same way that the well-known Carnot cycle is an idealization of physically realizable, *classical* processes or engines. There is evidence that the conventional Carnot cycle can be operated only between reservoirs at absolute temperatures of identical sign. No such restriction applies, however, to the quantum heat engine. Thus it may be used to calibrate negative absolute temperatures by relating them directly to positive temperatures. Negative efficiencies or efficiencies greater than unity have particularly simple interpretations in the quantum-heat-engine model. An important application of these concepts is in the calculation of optical *maser* parameters.

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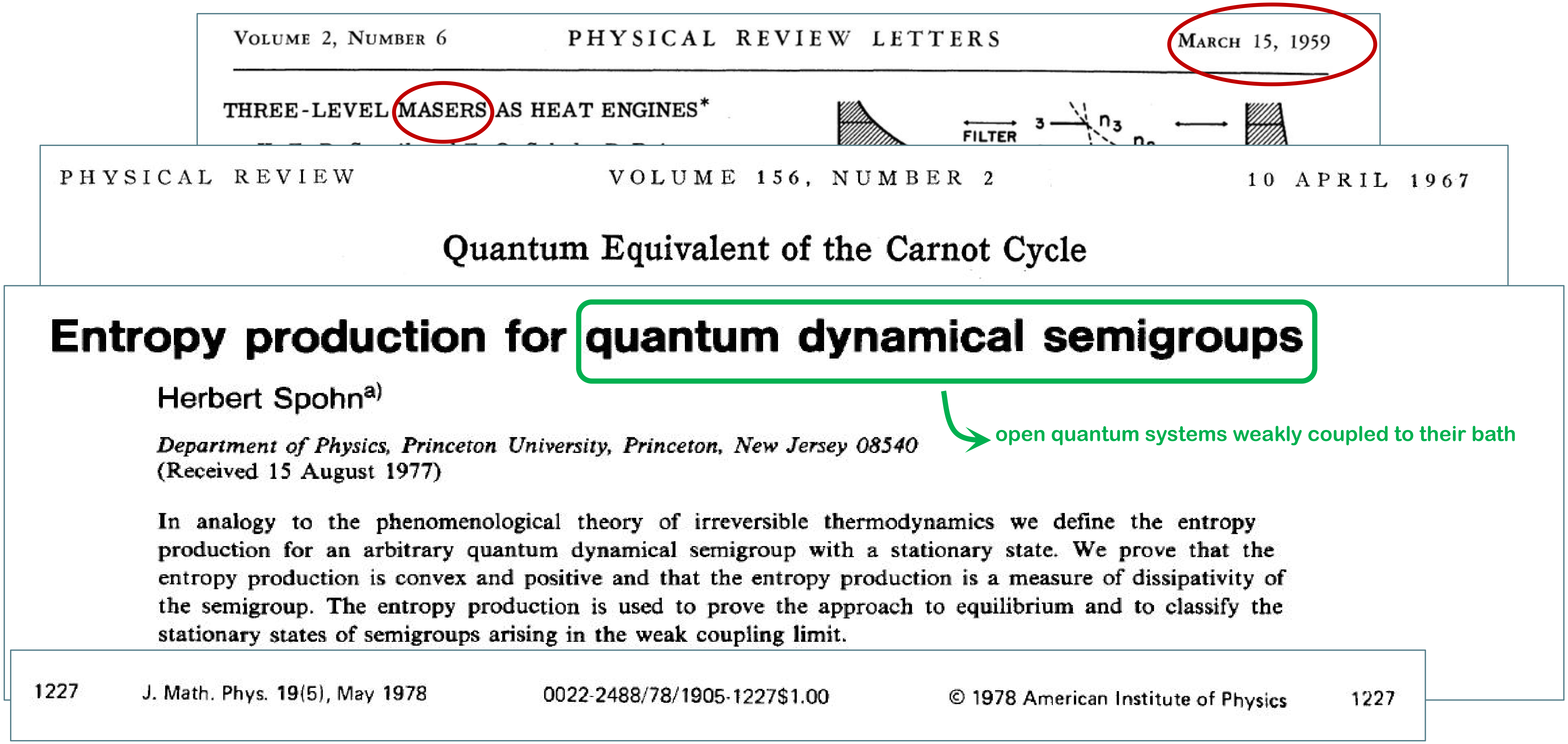

Volume 2, Number 6 PHYSICAL REVIEW LETTERS March 15, 1959

THREE-LEVEL MASERS AS HEAT ENGINES*

PHYSICAL REVIEW VOLUME 156, NUMBER 2 10 APRIL 1967

Quantum Equivalent of the Carnot Cycle

Entropy production for quantum dynamical semigroups

Herbert Spohn[a)]

Department of Physics, Princeton University, Princeton, New Jersey 08540
(Received 15 August 1977)

In analogy to the phenomenological theory of irreversible thermodynamics we define the entropy production for an arbitrary quantum dynamical semigroup with a stationary state. We prove that the entropy production is convex and positive and that the entropy production is a measure of dissipativity of the semigroup. The entropy production is used to prove the approach to equilibrium and to classify the stationary states of semigroups arising in the weak coupling limit.

open quantum systems weakly coupled to their bath

1227 J. Math. Phys. 19(5), May 1978 0022-2488/78/1905-1227$1.00 © 1978 American Institute of Physics 1227

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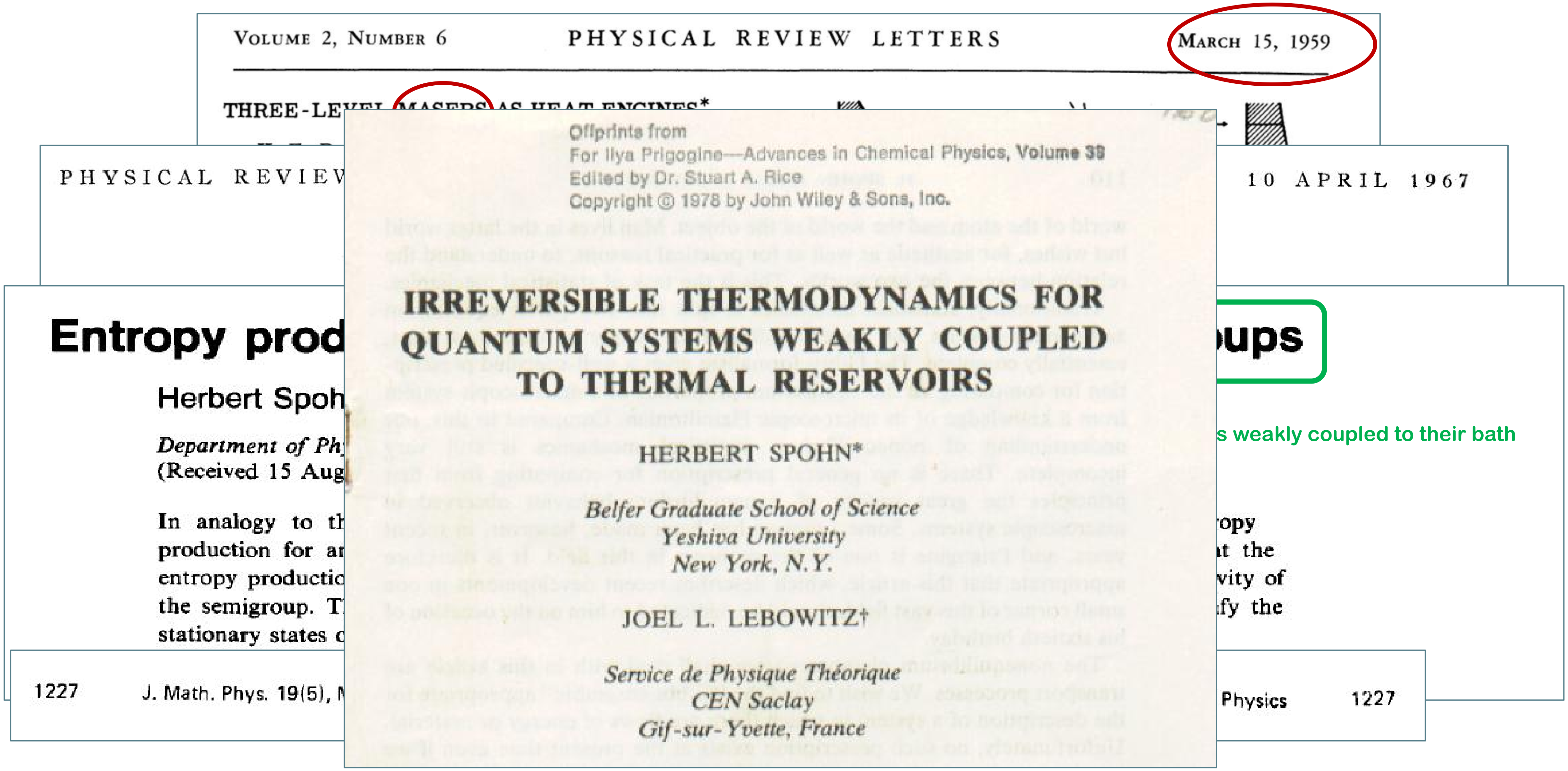

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IRREVERSIBLE THERMODYNAMICS FOR QUANTUM SYSTEMS WEAKLY COUPLED TO THERMAL RESERVOIRS

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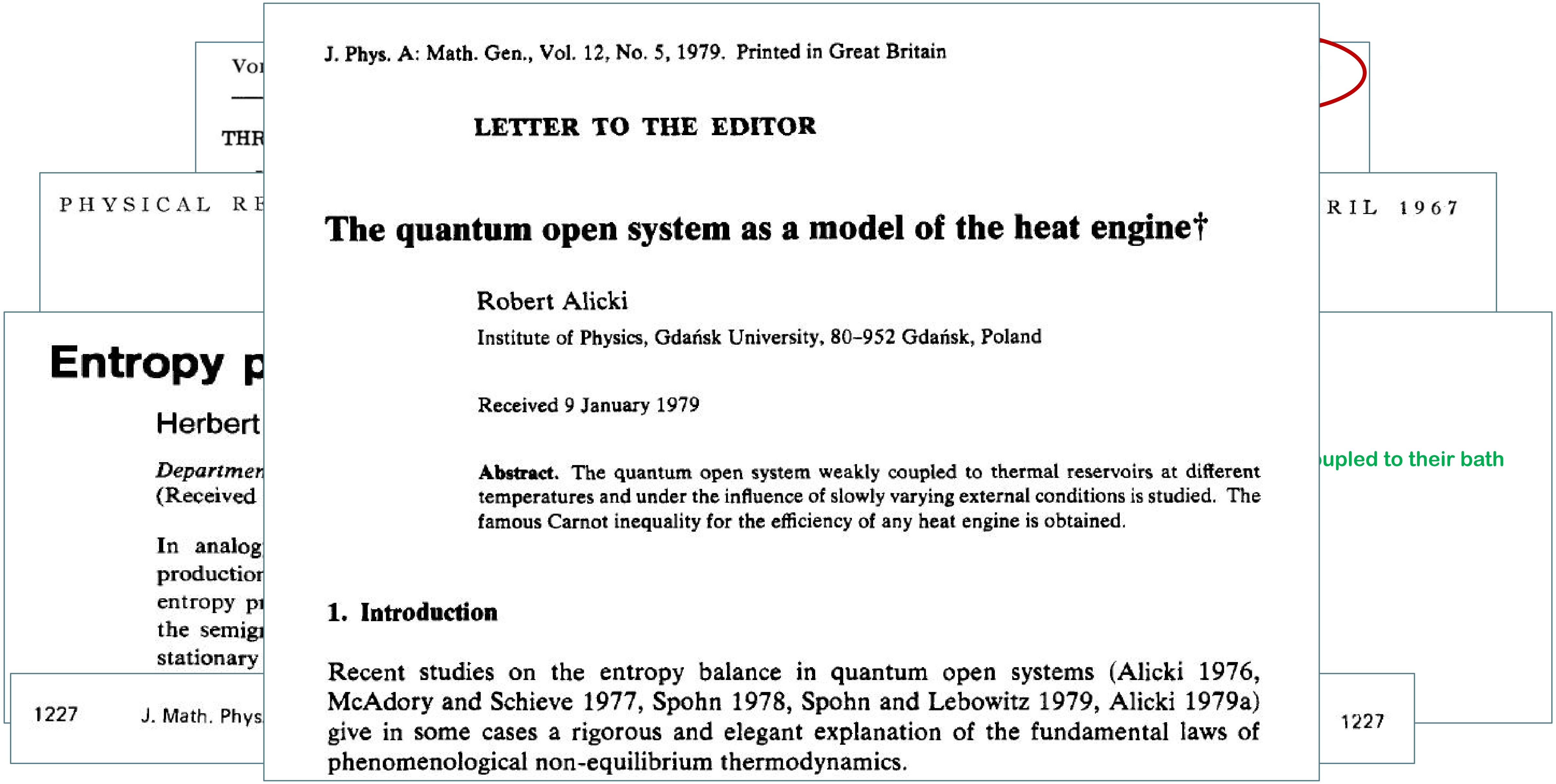

J. Phys. A: Math. Gen., Vol. 12, No. 5, 1979. Printed in Great Britain

LETTER TO THE EDITOR

The quantum open system as a model of the heat engine†

Robert Alicki

Institute of Physics, Gdańsk University, 80-952 Gdańsk, Poland

Received 9 January 1979

Abstract. The quantum open system weakly coupled to thermal reservoirs at different temperatures and under the influence of slowly varying external conditions is studied. The famous Carnot inequality for the efficiency of any heat engine is obtained.

1. Introduction

Recent studies on the entropy balance in quantum open systems (Alicki 1976, McAdory and Schieve 1977, Spohn 1978, Spohn and Lebowitz 1979, Alicki 1979a) give in some cases a rigorous and elegant explanation of the fundamental laws of phenomenological non-equilibrium thermodynamics.

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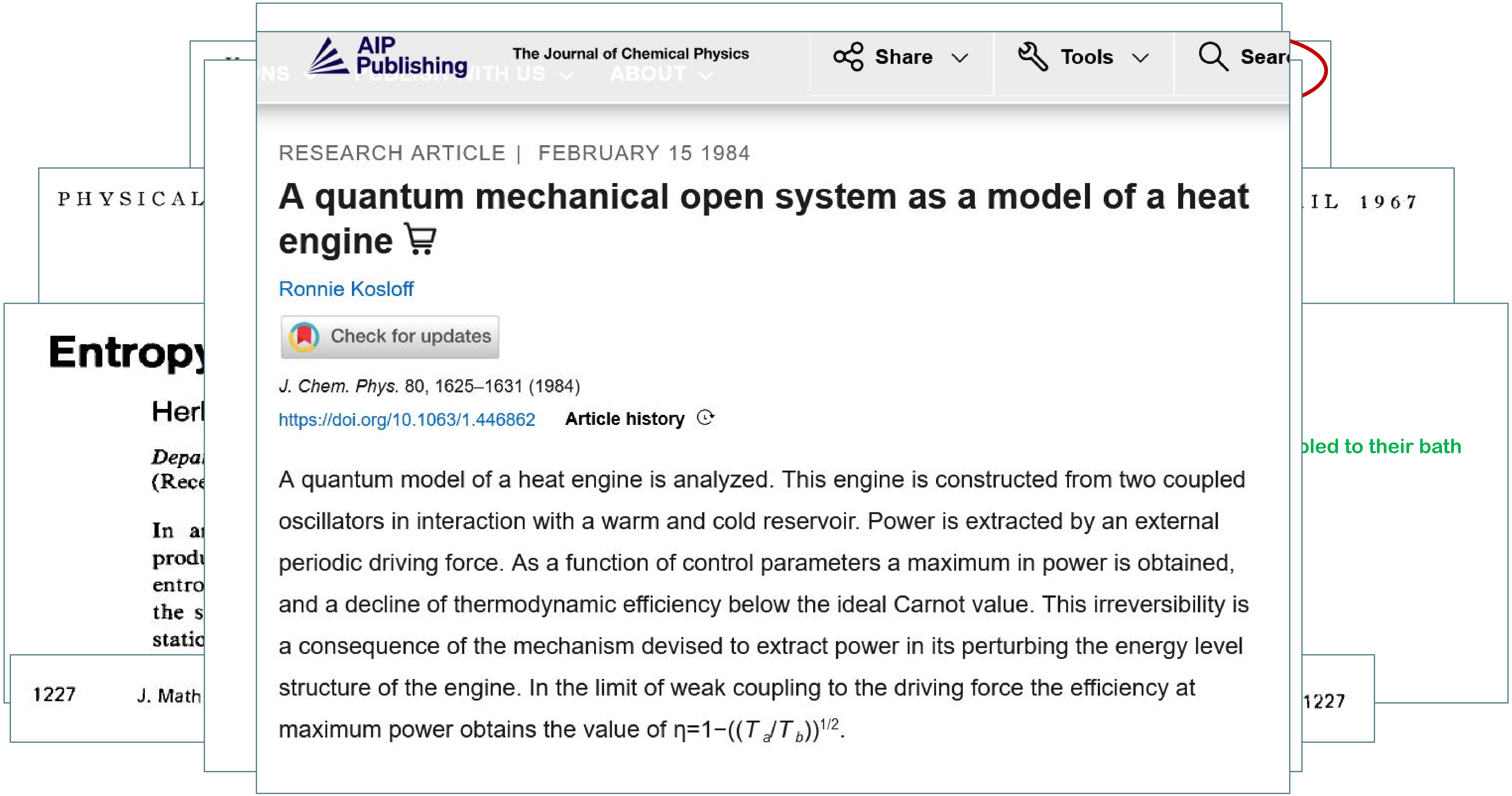

RESEARCH ARTICLE | FEBRUARY 15 1984

A quantum mechanical open system as a model of a heat engine

Ronnie Kosloff

Check for updates

J. Chem. Phys. 80, 1625–1631 (1984)

https://doi.org/10.1063/1.446862 **Article history**

A quantum model of a heat engine is analyzed. This engine is constructed from two coupled oscillators in interaction with a warm and cold reservoir. Power is extracted by an external periodic driving force. As a function of control parameters a maximum in power is obtained, and a decline of thermodynamic efficiency below the ideal Carnot value. This irreversibility is a consequence of the mechanism devised to extract power in its perturbing the energy level structure of the engine. In the limit of weak coupling to the driving force the efficiency at maximum power obtains the value of $\eta=1-((T_a/T_b))^{1/2}$.

I. Brief historical perspective

Brief historical perspective:

- First research articles on what will become Quantum Thermodynamics appeared from the years 1960 to 1980.

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- These pioneering papers provided the initial questions and research lines of quantum thermodynamics, which really started around 2000.

II. Current problematics of Quantum Thermodynamics

- Nowadays, the field evolved, with the emergence of several sub-fields, like:
    - Quantum advantages for quantum machines
    - Quantum advantage for quantum batteries
    - Work extraction from quantum systems and ergotropy
    - Thermal devices producing quantum resources (quantum coherence and entanglement)
    - Quantum clocks
    - Thermodynamic formalism beyond weak system-bath coupling
    - Entropy production and quantum origin of irreversibility
    - Autonomous Quantum thermodynamics
    - Stochastic Quantum Thermodynamics
    - Fluctuation Theorems
    - Control of fluctuations
    - Shortcut-to-adiabaticity
    - Quantum Thermometry
    - Thermalization in closed multipartite quantum systems
    - Resource Theory
    - Quantum Seep Limit
    - Thermodynamic Quantum Computing
    - Quantum Energetic
    - Third law of thermodynamics and Quantum Erasure

II. Current problematics of Quantum Thermodynamics

Current main objectives and aims of quantum Thermodynamics

- **Concept of Work and Heat at the quantum scale in a general context**
- **Entropy production for general quantum dynamics - quantum origin of irreversibility**
- **Trade-off between <u>performances of quantum operations</u> Versus <u>costs</u>**
  - ↳ **(fidelity, precision, velocity, robustness)**
  - ↳ **(energetic and thermodynamic cost)**
- **Energetic cost of information processing and its fundamental limits**
- **Understanding and then controling quantum fluctuations**

Quantum Thermodynamics aims to play for Quantum Technologies the same role as Thermodynamics played for the industrial revolution: optimize resources at hand in order to reach the best possible performances

Brief reminder about driven open quantum systems

Brief reminder about driven open quantum systems

(i) No quantum system can be perfectly isolated from their surrounding and environment.

- The interaction with this environment leads to *open dynamics*
- The environment is represented by a ***bath***
- A bath is usually a very large system with fixed properties, and often in a thermal state

(ii) Interaction with baths can be made on purpose: it is the essence of some operations like **quantum reset** and devices like **quantum heat engines** and **quantum refrigerators**.

(iii) Engineered interactions with baths can generate useful properties and states (entanglement, quantum coherences, squeezed states, etc)

→ 3 good reasons to study and analyse *driven open quantum systems*

when the system is driven by external control while interacting with a bath

Brief reminder about driven open quantum systems

❖ Driven systems

$$H_S(t) = \underbrace{H_0}_{\text{Free Hamiltonian of the system}} + \underbrace{V_{\mathrm{dr}}(t)}_{\text{contribution from external controls}}$$

Free Hamiltonian
of the system

contribution from
external controls

↳ results from interaction with
classial systems (or large
quantum systems behaving
effectively as classical ones)
(mainly lasers or
radio/microwaves-frequency
electromagnetic pulses)

- The dynamics generated by such time-dependent Hamiltonian is given by the Dyson serie

$$U_S(t) = \mathcal{T} e^{-\frac{i}{\hbar}\int_0^t dt' H_S(t')} := \sum_{n=0}^{+\infty} \frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \int_0^t dt_1 \int_0^t dt_2 \dots \int_0^t dt_n \mathcal{T} H_S(t_1) H_S(t_2) \dots H_S(t_n)$$

$$= \sum_{n=0}^{+\infty} \left(-\frac{i}{\hbar}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \dots \int_0^{t_{n-1}} dt_n H_S(t_1) H_S(t_2) \dots H_S(t_n)$$

Brief reminder about driven open quantum systems

A. Open dynamics

$$\underbrace{H_S(t)}_{\substack{\text{\textit{Local} Hamiltonian of the system} \\ \text{(free Hamiltonian + driving} \\ \text{Hamiltonian)}}} + \underbrace{V_{SB}(t)}_{\substack{\text{System-bath coupling} \\ \text{(potentially time-} \\ \text{dependent)}}} + \underbrace{H_B}_{\substack{\text{Free Hamiltonian} \\ \text{of the bath B}}}$$

→ Tracing out the bath: $\rho_S(t) := Tr_B[\rho_{SB}(t)]$ (= taking the partial trace over B)

Reduced dynamics of the system S:

$$\dot{\rho}_S(t) := \frac{d}{dt}\rho_S(t) = -\frac{i}{\hbar}\mathrm{Tr}_B\Big\{\big[H_S(t) + V_{SB}(t) + H_B, \rho_{SB}(t)\big]\Big\}$$

$$= \text{... lot of work ...}$$

$$= \underbrace{-\frac{i}{\hbar}[H(t), \rho_S(t)]}_{\text{Unitary part}} + \underbrace{\mathcal{D}_t[\rho_S(t)]}_{\substack{\text{Dissipative part (due to the} \\ \text{interaction with the bath)}}}$$

Observations:

- $H(t)$ can be different from $H_S(t)$ (due to the coupling with the bath). However, in the following, we will consider $H(t) = H_S(t)$.
- $\mathcal{D}_t$ is a ***superoperator*** (an operator acting on operators) and can be time-dependent. It is sometimes called the *dissipator* or *dissipative operator*.

Brief reminder about driven open quantum systems

B. General form of the dissipator

$$\mathcal{D}_t[\rho_S(t)] = \sum_k \gamma_k(t)\Big(L_k(t)\rho_S(t)L_k^\dagger(t) - \frac{1}{2}\underbrace{\{L_k^\dagger(t)L_k(t), \rho_S(t)\}}_{= L_k^\dagger(t)L_k(t)\rho_S(t) + \rho_S(t)L_k^\dagger(t)L_k(t)}\Big)$$

(anti-commutator: {A,B} := AB+BA)

- $L_k(t)$: *jump operator* or *Lindblad operator*

  ↳ generates ***quantum jumps***

- $\gamma_k(t)$: *decaying rate* or *jumping rate*

  $=$ probability per unit of time to have occurence of a ***quantum jump*** $L_k(t)$

  $=$ also related to the *equilibration timescale* since equilibration happens through sequences of many quantum jumps.

  - simple case: $\gamma_k(t) \geq 0$ for all t and k (=Markovian dynamics, no memory effects)
  - If there exists at least one k and t such that $\gamma_k(t) \leq 0$: presence of memory effects (non-Markovian dynamics)

Brief reminder about driven open quantum systems

❖ Exemple: two-level system (qubits, spins, atoms, etc)

master equation (for **weak coupling** with the bath)

$$\begin{aligned}\dot{\rho}_S(t) = -\frac{i}{\hbar}[H_S, \rho_S(t)] &+ \gamma_+\left(\sigma_+\rho_S(t)\sigma_- - \frac{1}{2}\{\sigma_-\sigma_+, \rho_S(t)\}\right) \\ &+ \gamma_-\left(\sigma_-\rho_S(t)\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho_S(t)\}\right) \\ &+ \frac{\gamma_z}{2}\left(\sigma_z\rho_S(t)\sigma_z - \rho_S(t)\right)\end{aligned}$$

$$H_S = \frac{\hbar\omega_s}{2}\sigma_z$$

with

$$\sigma_+ := |e\rangle\langle g| \qquad \sigma_- := |g\rangle\langle e| \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

→ $\gamma_k : \quad \gamma_+, \gamma_-, \gamma_z$ all positive

→ $$L_k : \quad \underbrace{\sigma_+}_{\text{jump from } |g\rangle \text{ to } |e\rangle}, \quad \underbrace{\sigma_-}_{\text{jump from } |e\rangle \text{ to } |g\rangle}, \quad \underbrace{\sigma_z}_{\text{not really a jump (but induces “dephasing” = loss of coherences)}}$$

Brief reminder about driven open quantum systems

One can show:

- **Population:**

$$\dot{p}_e(t) := \frac{d}{dt}\langle e|\rho_S(t)|e\rangle = \gamma_+ p_g(t) - \gamma_- p_e(t) = -\frac{1}{T_1} p_e(t) + \gamma_+ \quad \text{with} \quad T_1 := \frac{1}{\gamma_+ + \gamma_-}$$

$$\Longrightarrow \quad p_e(t) = e^{-t/T_1}\left[p_e(0) - \frac{\gamma_+}{\gamma_+ + \gamma_-}\right] + \frac{\gamma_+}{\gamma_+ + \gamma_-}$$

$\Longrightarrow$ **Population p_1 decays at a rate $1/T_1$**

- **Energy decay rate:**

$E_S(t) := \mathrm{Tr}[\rho_S(t) H_S] = \hbar\omega_s[p_e(t) - 1/2]$ follows $p_e(t)$ $\Longrightarrow$ **energy decays at a rate $1/T_1$**

- **Decoherence rate:**

$$c_{eg}(t) := \langle e|\rho_S(t)|g\rangle = e^{-i\omega_s t} e^{-t/T_2} c_{eg}(0) \quad \text{with} \quad T_2 := \left(\frac{\gamma_+ + \gamma_-}{2} + \gamma_z\right)^{-1}$$

$\Longrightarrow$ **coherence decays at a rate $1/T_2$**

Conclusion: **decaying rate**, **decoherence rate**, are determined by γ_+, γ_+ , and γ_z

Brief reminder about driven open quantum systems

❖ Observation:

- At long time, we have,

$$p_e(t=+\infty) = \frac{\gamma_+}{\gamma_+ + \gamma_-}$$

$$p_g(t=+\infty) = 1 - p_e(t=+\infty) = \frac{\gamma_-}{\gamma_+ + \gamma_-}$$

$$c_{eg}(t=\infty) = c_{ge}(t=\infty) = 0$$

- In situations of a thermal bath at temperature T_B with a weak system-bath coupling, we have: $\frac{\gamma_-}{\gamma_+} = e^{\frac{\hbar\omega_s}{k_B T_B}}$

- This implies: $\lim\limits_{t\to+\infty} \rho_S(t) = \rho_S^{\mathrm{th}}(T_B) := \underbrace{\frac{1}{Z} e^{-\frac{1}{k_B T_B} H_S}}$

thermal state

at temperature T_B

with $\left\{ \begin{array}{l} Z := e^{-\frac{\hbar\omega_s}{2k_B T}} + e^{\frac{\hbar\omega_s}{2k_B T}} \quad \text{partition function (normalization factor)} \\ k_B\text{: Boltzmann constant} \end{array} \right.$

$\Longrightarrow$ Conclusion: at **long times**, for **weak system-bath couplings**, the system S thermalizes at the bath's temperature T_B

Brief reminder about driven open quantum systems

C. Thermal state

❖ Definition

Let's consider a quantum system of Hamiltonian H

→ **Thermal state at temperature T:** $\rho^{\mathrm{th}}(T) := \dfrac{1}{Z} e^{-\frac{1}{k_B T} H}$

with $Z := \mathrm{Tr}\left[e^{-\frac{1}{k_b T} H}\right]$

Why?

- This state reproduces the definition/characteristics of classical thermal state
- This state is the state which maximizes the entropy (von Neumann entropy) at fixed energy.

Observations:

- In terms of the eigenvalues e_n and eigenstates $|e_n\rangle$ of H:

$$\rho^{\mathrm{th}}(T) = Z^{-1} \sum_n e^{-e_n/k_b T} |e_n\rangle\langle e_n| \quad \text{and} \quad Z = \sum_n e^{-e_n/k_b T}$$

- The quantity $\beta := \frac{1}{k_B T}$ is often used, and called the "inverse temperature".

Brief reminder about driven open quantum systems

D. Entropy of von Neumann

The **von Neumann entropy** associated with a density operator ρ is

$$S_{\mathrm{vN}}(\rho) = -\mathrm{Tr}(\rho \ln \rho)$$

- It is the generalization of the **Shanon entropy** (information theory) to quantum states
- For thermal states, the von Neumann entropy is equal to the thermodynamic entropy for classical systems:

$$S_{\mathrm{vN}}[\rho^{\mathrm{th}}(T)] = -\sum_n p_n \ln p_n \quad \text{with} \quad p_n = Z^{-1} e^{-e_n/k_B T} \text{ and } Z = \sum_n e^{-e_n/k_b T}$$

- Logarithm of an operator:

  For an operator A, $ln(A)$ is defined as the operator such that $exp[ln(A)] = A$

- $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ with $\langle\psi_i|\psi_j\rangle = \delta_{i,j} \Rightarrow S_{\mathrm{vN}}(\rho) = -\sum_i p_i \ln p_i$

- **Important property**: the von Neumann entropy is invariant by unitary transformation

$$S_{\mathrm{vN}}(U\rho U^\dagger) = S_{\mathrm{vN}}(\rho) \quad \text{for all unitary transformations U.}$$

Brief reminder about driven open quantum systems

E. Steady state

- For an open dynamics of the form

$$\dot{\rho}_S(t) = -\frac{i}{\hbar}[H_S, \rho_S(t)] + \sum_k \gamma_k \Big(L_k \rho_S(t) L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho_S(t)\} \Big)$$

$$:= \mathcal{L}[\rho_S(t)]$$

Time-independent

A **steady state** of the dynamics generated by $\mathcal{L}$ is a state ρ^{ss} such that:

$$\mathcal{L}[\rho^{ss}] = 0 \quad \Longrightarrow$$

If the system reaches ρ^{ss} at some instant of time t,
S will remain in this state at any later time

- In simple situations, ρ^{ss} is unique and is the **thermal state** at the **bath's temperature T**, $\rho^{th}(T)$

→ This is the case in at least 2 situations:

- when the coupling with the bath is weak and in the absence of memory effects
- when: $[L_k, H_S] = \omega_k L_k$ and $\gamma_k/\gamma_{k'} = e^{-(\omega_k - \omega_{k'})/k_B T}$ $\forall k, k'$

- If the generator $\mathcal{L}_t$ is **time-dependent**, one can define **instantaneous fixed states** as the state $\rho^{ss}(t)$ such that $\mathcal{L}_t[\rho^{ss}(t)] = 0$

Brief reminder about driven open quantum systems

→ Recap: In the following, we will consider quantum systems in diverse situations:

- A quantum system subject to external drive or control. This corresponds to a **unitary** dynamics described by a time-dependent Hamiltonian:

$$\dot{\rho}_S(t) = -\frac{i}{\hbar}[\rho_S(t), H_S(t)] \quad \text{with } H_S(t) \text{ typically of the form } \; H_S(t) = H_0 + V_{\mathrm{dr}}(t)$$

- A quantum system **weakly** interacting with a thermal bath. This corresponds to a non-unitary dynamics described by a GKSL master equation with time-independent Hamiltonian:

$$\dot{\rho}_S(t) = -\frac{i}{\hbar}[\underbrace{H_S}_{\text{time-independent}}, \rho_S(t)] + \underbrace{\sum_k \gamma_k \left(L_k \rho_S(t) L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho_S(t)\} \right)}_{\text{action of the bath}}$$

- A quantum system simultaneously subject to external drive and interacting with a bath. This corresponds to the most general dynamics, which is a non-unitary dynamics described by a GKLS master equation with time-dependent Hamiltonian

$$\begin{aligned} \dot{\rho}_S(t) &= -\frac{i}{\hbar}[H_S(t), \rho_S(t)] + \sum_k \gamma_k(t) \left(L_k(t) \rho_S(t) L_k^\dagger(t) - \frac{1}{2}\{L_k^\dagger(t) L_k(t), \rho_S(t)\} \right) \\ &= -\frac{i}{\hbar}[H_0 + \underbrace{V_{\mathrm{dr}}(t)}_{\text{action of the drive}}, \rho_S(t)] + \underbrace{\mathcal{D}_t[\rho_S(t)]}_{\text{action of the bath}} \qquad \text{with } \; H_S(t) = H_0 + V_{\mathrm{dr}}(t) \end{aligned}$$

→ Observations: such situations present all required ingredients for thermodynamics:

- External drive/control ≡ mechanical control in classical thermodynamics
- Interaction with thermal bath ≡ interaction with thermal bath in classical thermodynamics

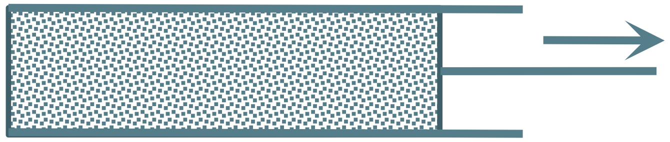
III. Concepts of work and heat

III. Concepts of work and heat

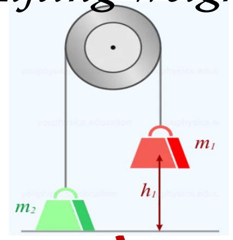
A. Classical concept of work:

- work ≈ energy “without uncertainty” ≈ “without noise” ≈ “mechanical energy”
- Examples of work exchange:

Displacement of a piston



Lifting weight



Generating Rotation

Generating electricity

Definition of work

$$\boxed{W = \vec{F}.\Delta\vec{r}}$$

Classical Mechanics

Resulting force applied on the system

Displacement of objects/ ensemble of particles

B. Classical concept of heat:

- Energy exchange associated with molecular excitation: random and disordered movements of molecules
- Energy exchange associated with change of entropy
- Disordered increase of kinetic energy:

average over all molecules of the ensemble/object/gas

$$\langle W\rangle = \langle\vec{F}.\Delta\vec{r}\rangle = 0$$

III. Concepts of work and heat

→ Extension to classical stochastic thermodynamics

K. Sekimoto: Stochastic Energetics, Springer (2010)

Context:

- Single particle in contact with a thermal bath (= ensemble of other particules globally in a thermal state)

→ canonical coordinates: (q,p)

- Deterministic part of the dynamics is described by the classical Hamiltonian (Hamilton's equation of motion)

→ $H_\lambda(q,p)$

λ: parametrizes the external forces acting on the system (external field and or confining potentials)

- Non-deterministic (or stochastic) part of the dynamics is induced by the interaction with the bath → described by stochastic terms "a la Langevin"

- Infinitesimal energy variation:

$$\frac{dH_\lambda(p,q)}{dt} = \underbrace{\dot{\lambda}\frac{\partial H_\lambda(p,q)}{\partial \lambda}}_{\substack{\text{Energy change due}\\ \text{to external forces}\\ \Downarrow\\ \dot{W}}} + \underbrace{\dot{q}\frac{\partial H_\lambda(p,q)}{\partial q} + \dot{p}\frac{\partial H_\lambda(p,q)}{\partial p}}_{\substack{\text{Energy change due to interaction}\\ \text{with thermal bath (reduces to zero if}\\ \text{no bath interaction)}\\ \Downarrow\\ \dot{Q}}}$$

III. Concepts of work and heat

C. Work for quantum systems

We consider a quantum system S described by a density operator $\rho_S(t)$ and Hamiltonian H_S(t), and **weakly** interacting with a thermal bath. The resulsting dynamics is assumed to be of the form:

$$\frac{d}{dt}\rho_S(t) = -\frac{i}{\hbar}[H_S(t), \rho_S(t)] + \underbrace{\mathcal{D}_t[\rho_S(t)]}$$

describes the action of the bath

Work for quantum systems is:

- Exchange of energy "without uncertainty" ≈ "without noise"

  $\Rightarrow$ Exchange of energy without change of entropy

- Change of energy due to external controls

- Substituting $\boldsymbol{H_\lambda(p,q)}$ by $\boldsymbol{Tr[\rho_S(t)H_S(t)]}$ in the classical stochastic definition of work, one gets:

→ $$\dot{W}_S(t) := \mathrm{Tr}[\rho_S(t)\underbrace{\dot{H}_S(t)}]$$

Infinitesimal work exchange

variation of the Hamiltonian due to variation of external parameters

→ $$W_S(t) = \int_0^t du \mathrm{Tr}[\rho_S(u)\dot{H}_S(u)]$$

Finite work exchange

→ *Observation: we recover the proterty that work exchange is induced by external control or mechanical action, because in Quantum Mechanics time-dependent Hamiltonians are consequences of external controls (like systems driven by laser, magnetic fileds, etc.)*

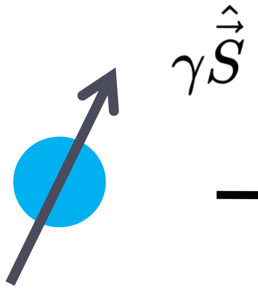
III. Concepts of work and heat

- Example: spin-1/2

  Elementary particles have **intrinsic angular momentum**, $\longrightarrow \hat{\vec{S}}$

  which gives rise to **intrinsic magnetic moment** through the gyromagnetic factor $\boldsymbol{\gamma}$

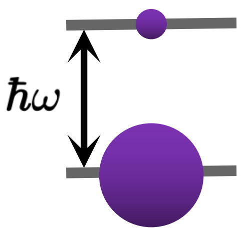
  $\hookrightarrow \hat{\vec{M}} = \gamma\hat{\vec{S}}$



$$\longrightarrow \quad \hat{H} = -\gamma\hat{\vec{S}}.\vec{B}$$

(quantized classical potential energy $E_P = -\vec{M}.\vec{B}$)

→ **2 quantized energy levels** $\begin{cases} E_+ = \dfrac{\hbar\omega}{2} \\ E_- = -\dfrac{\hbar\omega}{2} \end{cases}$ with $\omega = \gamma|\vec{B}|$ →

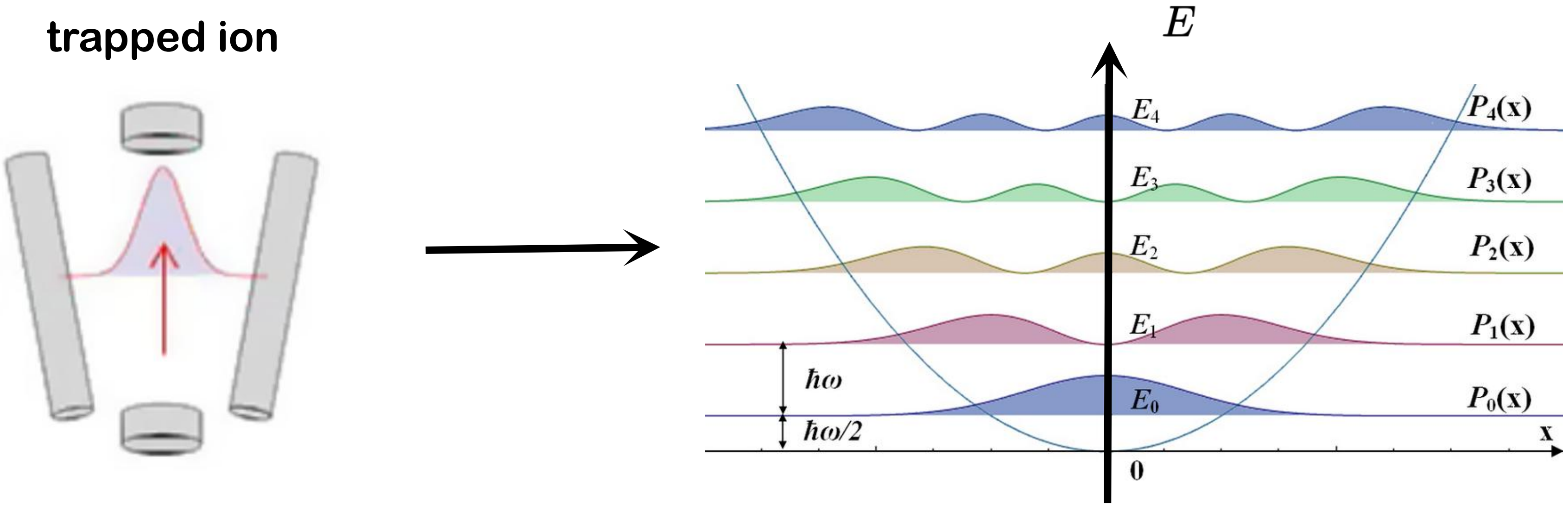


→ According to the definition of the previous slide, work exchanges correspond to variation of Hamiltonian $\Longrightarrow$ **Applying work = varying the magentic field intensity** $\Longrightarrow$ **Applying work = increasing $(W \geq 0)$ or decreasing $(W \leq 0)$ the energy levels**

→ $\dot{W}(t) = -\gamma \mathrm{Tr}\left[\rho_S(t)\hat{\vec{S}}.\dot{\vec{B}}(t)\right]$ and $W(t) = -\gamma\int_0^t du \mathrm{Tr}\left[\rho_S(u)\hat{\vec{S}}.\dot{\vec{B}}(u)\right]$

III. Concepts of work and heat

- Example: quantum harmonic oscillator



Quantum particle in a harmonic potential $V = \frac{1}{2}kx^2$

→ **Hamiltonian** $\hat{H} = \frac{\hat{P}^2}{2m} + \frac{1}{2}k\hat{X}^2 = \frac{\hat{P}^2}{2m} + \frac{1}{2}m\omega^2\hat{X}^2$

$$\omega = \sqrt{k/m}$$

Quantized energy levels: $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$

→ According to the definition of previous slides, work exchanges correspond to variation of Hamiltonian $\Longrightarrow$ **Applying work = varying the trap stiffness k**

→ $\dot{W}(t) = \frac{1}{2}\dot{k}(t)\mathrm{Tr}\left[\rho_S(t)\hat{X}^2\right]$ and $W(t) = \frac{1}{2}\int_0^t du\, \dot{k}(u)\mathrm{Tr}\left[\rho_S(u)\hat{X}^2\right]$

III. Concepts of work and heat

D. Heat for quantum systems:

- Variation of energy associated with changes of entropy
- Change of energy due to interaction with the thermal bath
- Substituting $\boldsymbol{H_\lambda(p,q)}$ by $\boldsymbol{Tr[\rho_S(t)H_S(t)]}$ in the classical stochastic definition of heat, one gets:

$$\longrightarrow \quad \dot{Q}_S(t) := \mathrm{Tr}[\underbrace{\dot{\rho}_S(t)}H_S(t)]$$

Infinitesimal heat exchange

variation of the state of the system due to interaction with the thermal bath

(for weak coupling with the bath)

$$\longrightarrow \quad Q_S(t) := \int_0^t du \mathrm{Tr}[\dot{\rho}_S(u)H_S(u)]$$

Finite heat exchange

❖ *Exercise*: using the dynamics $\dot{\rho}_S(t) = -\frac{i}{\hbar}[H_S(t), \rho_S(t)] + \mathcal{D}_t[\rho_S(t)]$ show that $\dot{Q}_S(t) = \underbrace{\mathrm{Tr}\Big[\mathcal{D}_t[\rho_S(t)]H_S(t)\Big]}$

changes of energy induced by the bath

→ *Observation*: we recover the analogy with classical heat exchanges, where heat exchanges are induced by energy exchanges with thermal baths.

III. Concepts of work and heat

E. Total energy and first law for quantum systems

- Total energy of S: $E_S(t) := \mathrm{Tr}[\rho_S(t)H_S(t)]$

$$\longrightarrow \quad \dot{E}_S(t) := \underbrace{\mathrm{Tr}[\dot{\rho}_S(t)H_S(t)]}_{\dot{Q}_S(t)} + \underbrace{\mathrm{Tr}[\rho_S(t)\dot{H}_S(t)]}_{\dot{W}_S(t)}$$

Finite variation : $$\Delta E_S = \underbrace{\int_0^t du\mathrm{Tr}[\dot{\rho}_S(u)\hat{H}_S(u)]}_{Q_S(t)} + \underbrace{\int_0^t du\mathrm{Tr}[\rho_S(u)\dot{\hat{H}}_S(u)]}_{W_S(t)}$$

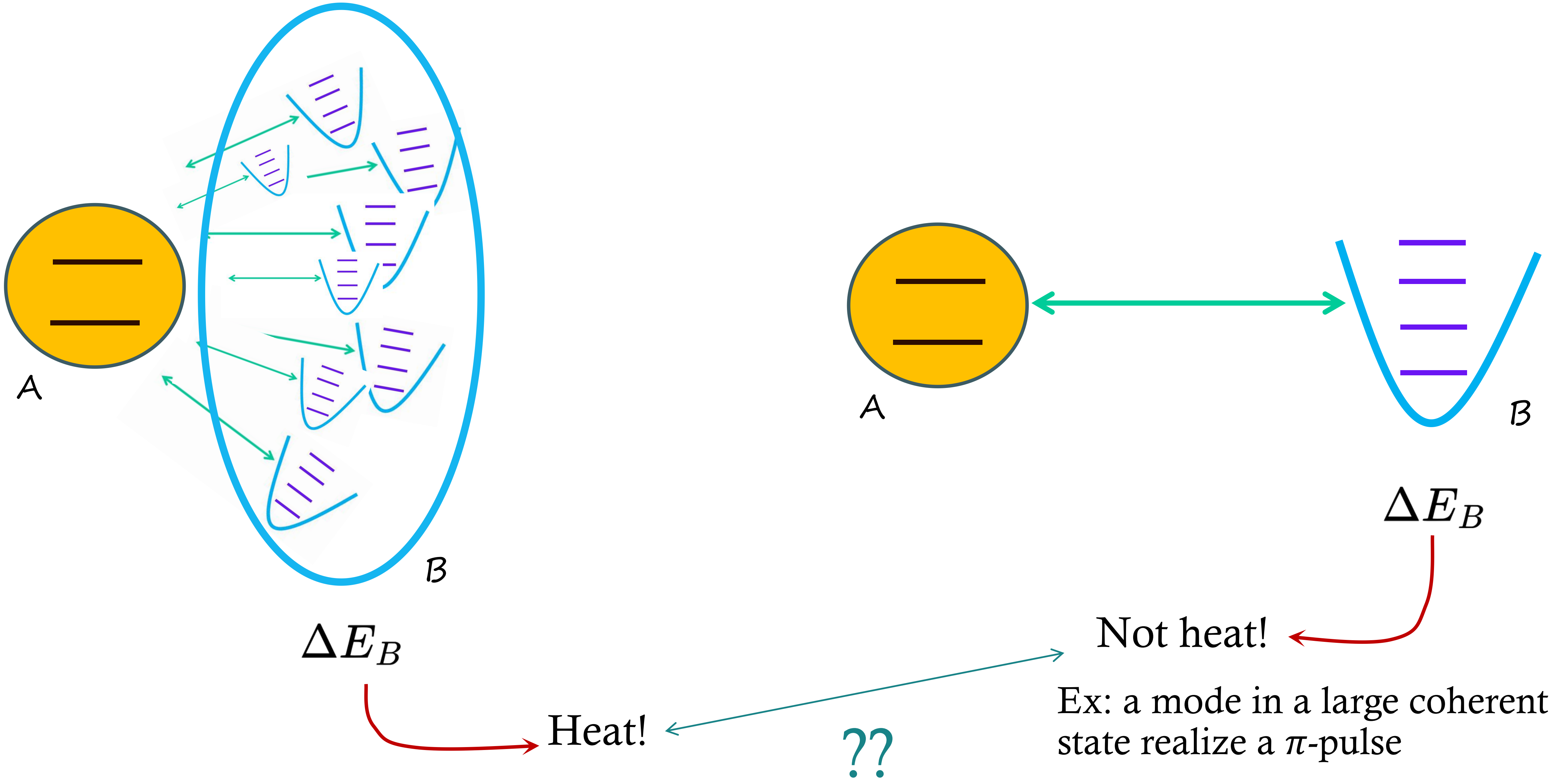
→ **Fisrt Law of Thermodynamics!**

- Important to keep in mind:
  - ❖ Dynamics with no external drive: $W_S(t) = 0$
  - ❖ Dynamics with no interaction with the bath: $Q_S(t) = 0$
  - ❖ General dynamics: $W_S(t) \neq 0$ and $Q_S(t) \neq 0$

III. Concepts of work and heat

F. Limitations

- Non-thermal bath and/or finite bath
  - ❖ Why does the energy provided by the bath should always be heat?



ΔE_B

Heat!

ΔE_B

Not heat!

??

Ex: a mode in a large coherent state realize a π-pulse

Observation: the quantum system of interest is sometimes called S, and sometimes A. This is just a small confusion in the notation which has to be ignored: $S \equiv A$

Side notes

In this side note, we show that an harmonic oscillator B in a large coherent state tends to induce, on a short timescale, a time-dependent componant in the Hamiltonian of the qubit A.

$$H_{AB} = \frac{\hbar\omega_A}{2}\sigma_z + g\sigma_x(a^\dagger + a) + \hbar\omega_B a^\dagger a$$

General situation:

(valid for any system A and B)

$$H_{AB} = H_A + X_A \otimes X_B + H_B$$

$$\dot{\rho}_{AB} = -i[H_{AB}, \rho_{AB}(t)] \qquad (\hbar \equiv 1)$$

$$\dot{\rho}_A(t) = -i\mathrm{Tr}_B\{[H_{AB}, \rho_{AB}(t)]\}$$

$$\dot{\rho}_A(t) = -i[H_A, \rho_A(t)] - ig\underbrace{\mathrm{Tr}_B\{[X_A \otimes X_B, \rho_{AB}(t)]\}} - i\mathrm{Tr}_B\{\cancel{[H_B, \rho_{AB}(t)]}\} \quad = 0$$

If we neglect the correlations between A and B:

$$\rho_{AB}(t) \simeq \mathrm{Tr}_B\{\rho_{AB}(t)\} \otimes \mathrm{Tr}_A\{\rho_{AB}(t)\} = \rho_A(t) \otimes \rho_B(t)$$

$$\begin{aligned}\mathrm{Tr}_B\{[X_A \otimes X_B, \rho_A(t) \otimes \rho_B(t)]\} &= \mathrm{Tr}_B\{X_A \otimes X_B \rho_A(t) \otimes \rho_B(t)\} - \mathrm{Tr}_B\{\rho_A(t) \otimes \rho_B(t) X_A \otimes X_B\} \\ &= X_A \rho_A(t) \mathrm{Tr}_B\{X_B \rho_B(t)\} - \rho_A(t) X_A \mathrm{Tr}_B\{\rho_B(t) X_B\} \\ &= [x(t) X_A, \rho_A(t)] \qquad \text{with } x(t) = \mathrm{Tr}_B\{\rho_B(t) X_B\} = \mathrm{Tr}_B\{X_B \rho_B(t)\}\end{aligned}$$

Side notes (end)

Conlcusion:

$$\dot{\rho}_A(t) = -i[H_A + g x(t) X_A, \rho_A(t)]$$

neglecting correlations between A and B

→ We obtain that neglecting the correlations between A and B results in: (i) a unitary dynamics for A; (ii) an effective Hamiltonian with a time-dependent component x(t) determined by the time evolution of B.

→ However, one has to be careful: we made a big approximation, we neglected the correlations between S and B. **This is a resonable approximation only on short timescales** ($t \ll g^{-1}$) and when the state of B is very energetic and not affected by the influence of B. If one is interested in long time behavior, one has to consider correlations between A and B including for instance higher order contributions.

For the harmonic oscillator:

$$x(t) = \mathrm{Tr}_B\{\rho_B(t) X_B\} = \mathrm{Tr}_B\{\rho_B(t)(a^\dagger + a)\}$$

$$\rho_B(t) \simeq e^{-iH_B t} \rho_B(0) e^{iH_B t}$$

(we approximate the time evolution of B by its free evolution. This is valid only on a short timescale, for $t \ll g^{-1}$)

$\rho_B(0) = |\alpha_0\rangle\langle\alpha_0|$ coherent state

$$x(t) = \alpha_0^* e^{i\omega_B t} + \alpha_0 e^{-i\omega_B t}$$

III. Concepts of work and heat

- Strong coupling
  - ❖ How to take into account the coupling energy?

$$\Delta E_{AB} = \Delta E_A + \underbrace{\Delta E_{\text{interaction}}} + \Delta E_B$$

$$= \mathrm{Tr}[\rho_{AB}(t) V_{AB}(t)] - \mathrm{Tr}[\rho_{AB}(0) V_{AB}(0)]$$

Work or Heat?

Does it contribute to the energy A or B?

IV. Opening: state of current research

A. Strong coupling

(M. Esposito, K. Lindenberg, C. Van den Broeck, Entropy production as correlation between system and reservoir, New J Phys 12, 013013 (2010))

Isolated, global unitary evolution U_{AB}

Hypothesis: - B is initially in a thermal state
- A and B are initially uncorrelated

→ Heat: $Q_A(t) = -\Delta E_B$ → All energy exchanged with the bath is heat

→ Justification through entropy production:

$$\Sigma_A(t) = \underbrace{\Delta S_A}_{\text{Variation of von Neumann entropy of A}} - \beta_B Q_A(t) \geq 0$$

(Clasius inequality extended to quantum system)

IV. Opening: state of current research

→ For the work, still

$$W_A(t) := \int_0^t du \mathrm{Tr}[\rho_A(u)\dot{H}_A(u)]$$

→ Then, we can show

$$W_A(t) + Q_A(t) = \Delta E_A + \Delta E_{\text{int}}$$

$$\Delta E_A := \mathrm{Tr}[\rho_A(t)H_A(t)] - \mathrm{Tr}[\rho_A(0)H_A(0)]$$

$$\Delta E_{\text{int}} := \mathrm{Tr}[\rho_{AB}(t)V_{AB}] - \mathrm{Tr}[\rho_{AB}(0)V_{AB}]$$

→ Conclusion: the interaction energy is included in the energy decomposition of heat and work

IV. Opening: state of current research

B. Autonomous thermodynamics

(C. Elouard, C. Lombard Latune: Extending the Laws of Thermodynamics for Arbitrary Autonomous Quantum Systems. PRX Quantum 4, 020309 (2023))

Isolated, global unitary evolution U_{AB}

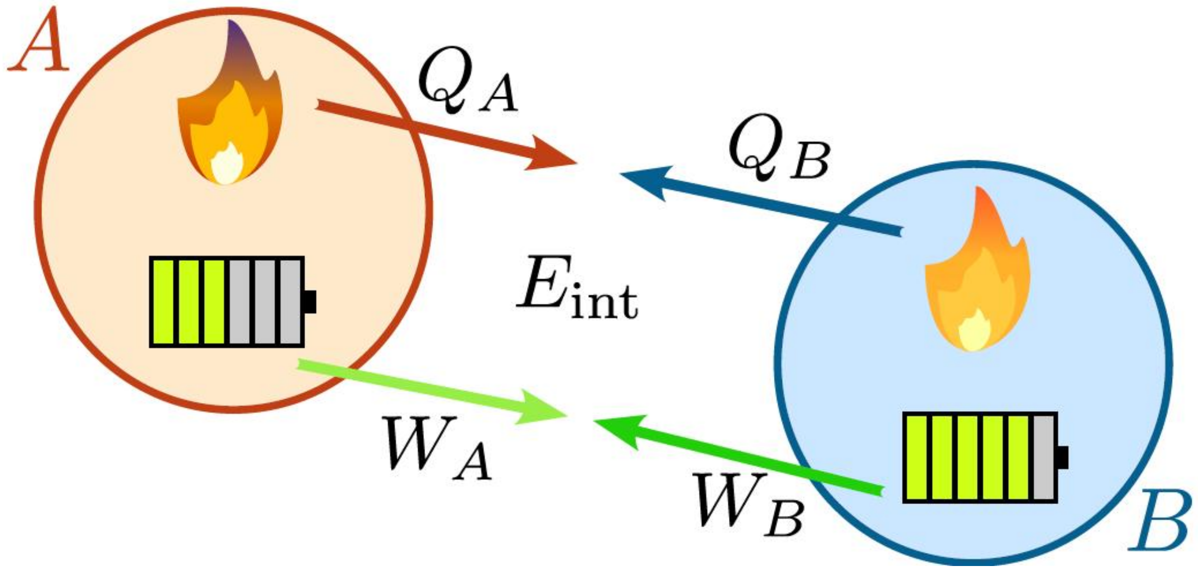
Hypothesis: A and B are initially uncorrelated

- The energy of A (B) is divided into:

a $\underbrace{\text{thermal energy}}_{E_A^{\text{th}}}$ (noisy energy) and a $\underbrace{\text{non-thermal energy}}_{\mathcal{E}_A}$ ("unitary" energy)

- $Q_A = -\Delta E_A^{th}$: heat provided by A
- $Q_B = -\Delta E_B^{th}$: heat provided by B
- $W_A = -\Delta \mathcal{E}_A$: work provided by A
- $W_B = -\Delta \mathcal{E}_B$: work provided by B

IV. Opening: state of current research



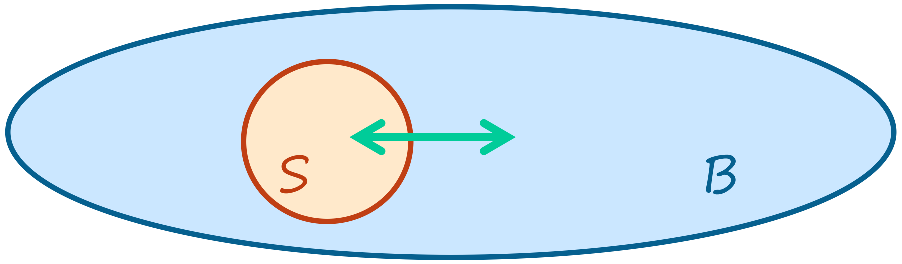
- $Q_A = -\Delta E_A^{th}$: heat provided by A
- $W_A = -\Delta \mathcal{E}_A$: work provided by A
- $Q_B = -\Delta E_B^{th}$: heat provided by B
- $W_B = -\Delta \mathcal{E}_B$: work provided by B

$$\rightarrow \begin{cases} \Sigma_A = \Delta S_A - \beta_B Q_B \geq 0 \\ \Sigma_B = \Delta S_B - \beta_A Q_A \geq 0 \end{cases}$$

IV. Opening: state of current research

C. Minimal dissipator framework

A. Colla, H.-P. Breuer: Open-system approach to nonequilibrium quantum thermodynamics at arbitrary coupling. Phys. Rev. A 105, 052216 (2022)



Arbitrary quantum system S coupled to a bath B

$$\underbrace{H_{SB} = H_S + V_{SB} + H_B \qquad \rho_{SB}(0) = \rho_S(0) \otimes \rho_B(0)}$$

Tracing out the bath

Hypothesis:
- S and B are initially uncorrelated
- B is an infinite bath

$$\rho_S(t) = \Lambda_t \rho_S(0)$$

CPTP map

$$\mathcal{L}_t = \dot{\Lambda}_t \Lambda_t^{-1}$$

If the inverse exists

$$\dot{\rho}_S(t) = \mathcal{L}_t \rho_S(t)$$

Master Equation

(requirement of Hermiticity and trace preservation)

$$\rho_S(t) = \underbrace{-i[K_S(t), \rho_S(t)]}_{\mathcal{H}} + \underbrace{\sum_k \gamma_k(t) \left[L_k(t) \rho_S(t) L_k^\dagger(t) - \frac{1}{2} \{ L_k^\dagger(t) L_k(t), \rho_S(t) \} \right]}_{\mathcal{D}}$$

Time convolutionless master equation

Important obs: $K_S(t) \neq H_S$ contains Lamb shift, energy renormalization, etc...

→ operator associated with the physical energy of S

IV. Opening: state of current research

The plan: → $E_S(t) := \mathrm{Tr}[\rho_S(t) K_S(t)]$ → $\begin{cases} \dot{Q}_S(t) := \mathrm{Tr}[\dot{\rho}_S(t) K_S(t)] \\ \dot{W}_S(t) := \mathrm{Tr}[\rho_S(t) \dot{K}_S(t)] \end{cases}$

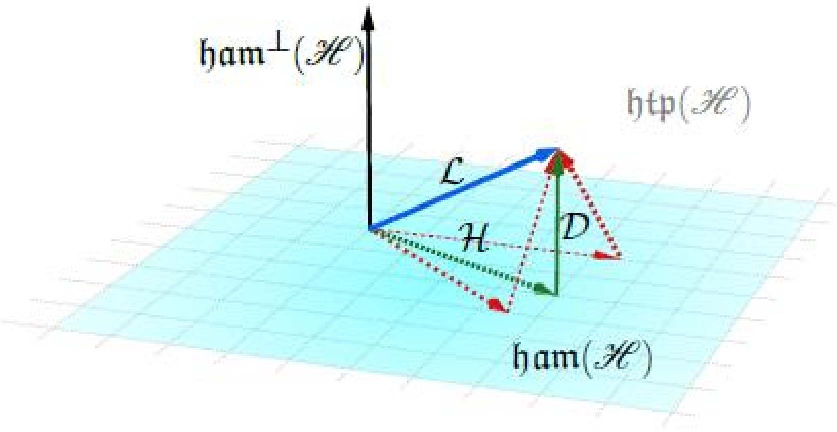
- ❖ Problem: the form of the master equation is not unique

$$L_k(t) \to L_k(t) - \alpha_k(t)\mathbb{I}$$

$$K_S(t) \to K_S(t) + \sum_k \frac{\gamma_k(t)}{2i}\Big[\alpha_k(t) L_k^\dagger(t) - \alpha_k^*(t) L_k(t)\Big] + \beta(t)\mathbb{I}$$

- ❖ Solution: minimal dissipator

$$\langle \mathcal{L}_1, \mathcal{L}_2 \rangle = \overline{\langle \psi | \overline{\mathcal{L}_1\big[\,|\phi\rangle\langle\phi|\,\big] \mathcal{L}_2\big[\,|\phi\rangle\langle\phi|\,\big]} |\psi\rangle}$$



→ Unique (mathematical) way to define $K_S(t)$

(Obs: the dissipator of minimal norm is composed of traceless jump operators)

IV. Opening: state of current research

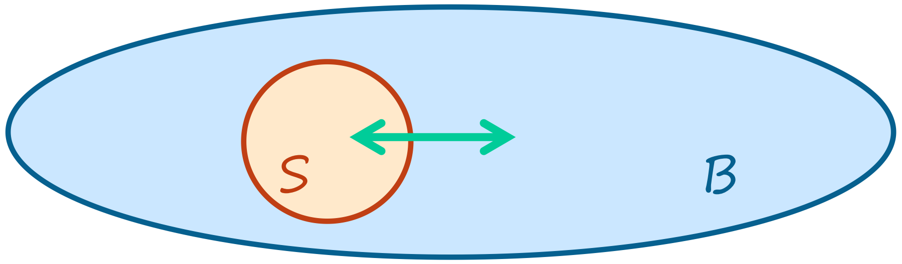
→ Then, “usual” defintions (with the dissipator of minimal norm and associated unitary operator)

$$\begin{cases} E_S(t) := \mathrm{Tr}[\rho_S(t) K_S(t)] \\ \dot{Q}_S(t) := \mathrm{Tr}[\dot{\rho}_S(t) K_S(t)] \\ \dot{W}_S(t) := \mathrm{Tr}[\rho_S(t) \dot{K}_S(t)] \end{cases}$$

IV. Opening: state of current research

D. Hamiltonian of Mean Force Gibbs

P. Strasberg, Phys. Rev. Lett. 123, 180604 (2019)
Á. Rivas,. Phys. Rev. Lett. 124, 160601 (2020)



Hypothesis: - S and B are initially uncorrelated
- B is an infinite bath

$$H_{SB} = H_S + V_{SB} + H_B$$

→ Mean force Gibbs state:

$$\rho_S^{MFG} := \mathrm{Tr}_B[e^{-\beta H_{SB}} / \mathrm{Tr}_{SB}[e^{-\beta H_{SB}}]]$$

(takes into account contributions from V_{SB})

→ Hamiltonian of Mean force:

$$H_S^{MFG} := -\beta^{-1} \ln \left(\frac{Z_{SB}}{Z_B} \rho_S^{MFG} \right)$$

→ Thermodynamic framework based on H_S^{MFG}

Energy of S: $E_S(t) = \mathrm{Tr}_S[\rho_S(t) H_S^{MFG}]$

IV. Opening: state of current research

E. Additional frameworks

- Separated role of coherences

❖ B. d. L. Bernardo: Unraveling the role of coherence in the first law of quantum thermodynamics. Phys. Rev. E 102, 062152 (2020)

❖ A. Vallejo, A. Romanelli, V. Feldman, R. Donangelo: Evolution of expected values in open quantum systems. Phys. Rev. A 111, 032201 (2025)

- Work operator

❖ A. E. Allahverdyan, Th. M. Nieuwenhuizen: Fluctuations of work from quantum subensembles: The case against quantum work-fluctuation theorems. Phys. Rev. E 71, 066102 (2005)

❖ T. A. B. Pinto Silva, D. Gelbwaser-Klimovsky: Quantum work: Reconciling quantum mechanics and thermodynamics. Phys. Rev. Res. 6, 2 (2024)

- Question and debate around work fluctuation (see mroe details in lecture III)

❖ M. Perarnau-Llobet, E. Bäumer, K. V. Hovhannisyan, M. Huber, A. Acin: No-Go Theorem for the Characterization of Work Fluctuations in Coherent Quantum Systems. Phys. Rev. Lett. 118, 070601 (2017)

❖ T. A. B. Pinto Silva, D. Gelbwaser-Klimovsky: Quantum work: Reconciling quantum mechanics and thermodynamics. Phys. Rev. Res. 6, 2 (2024)

Recap

Recap on heat and work

- Heat for quantum systems is intimately related to interaction with external degrees of freedom and change of local entropy
- Work for quantum systems is intimately related to classical control and unitary transformation (coherent energy exchange)
- For weak coupling, with infinite thermal bath, all definitions converge to the one given at the beginning of the lecture:

$$Q_S(t) = \int_0^t du \mathrm{Tr}[\dot{\rho}_S(u) H_S(u)]$$

$$W_S(t) = \int_0^t du \mathrm{Tr}[\rho_S(u) \dot{H}_S(u)]$$

- For strong coupling: contributions from interaction energy have to enter the game → how it is taken into account depends on the framework
  - ❖ Esposito, Lindenberg, Van den Broeck
  - ❖ Colla and Breuer
  - ❖ Mean force Hamiltonian
- For finite bath, the evolution of the state of the bath has to be taken into account
  - ❖ Esposito, Lindenberg, Van den Broeck
  - ❖ Elouard and Latune
- Which framework is the more accurate? → Still debated, most probably depends on the context

Recap on the open quantum system part

- Open quantum dynamics are described in term of "**dissipators**" or "**dissipative operators**", $\mathfrak{D}_t$.

- Dissipative operators contains **jump operators** L_k promoting ***quantum jumps*** at rate determined by the coefficients γ_k, the **jumping rates**.

- At long time, the succession of ***quantum jumps*** leads to decoherence and energy decay, and eventually to thermalization at the bath's temperature.

- Notions of **information** (S_{nV}), **work** (W), and **heat** (Q) can be defined in the quantum regime. From the fundamental point of view, they are central to analyse the intimate relation between energy and information in the quantum regime. From a practical perspective, they are crucial to analyse, understand, and enhance the performances of quantum operations.