Introduction to quantum thermodynamics
An open systems perspective

Dr Graeme Pleasance

Quantum@SUN group
Department of Physics
Stellenbosch University

NITheCS Mini-School
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Stellenbosch UNIVERSITY IYUNIVESITHI UNIVERSITEIT

NITheCS National Institute for Theoretical and Computational Sciences

QSUN Quantum Research Group of Stellenbosch University

Contents

Background

Macroscopic thermodynamics: phenomenological theory describing the *average* behavior of heat, work and entropy.

Quantum thermodynamics: extends 'classical' concepts of heat and work into the microscopic domain.

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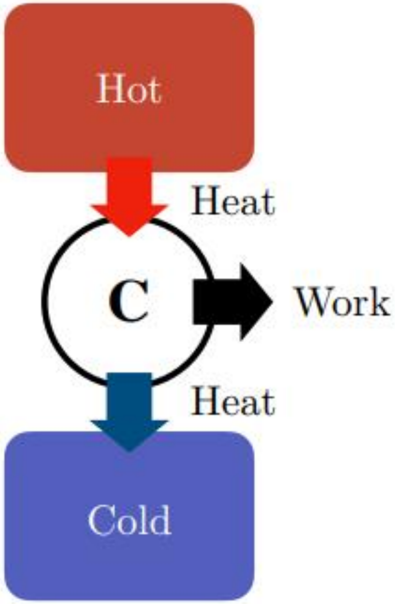

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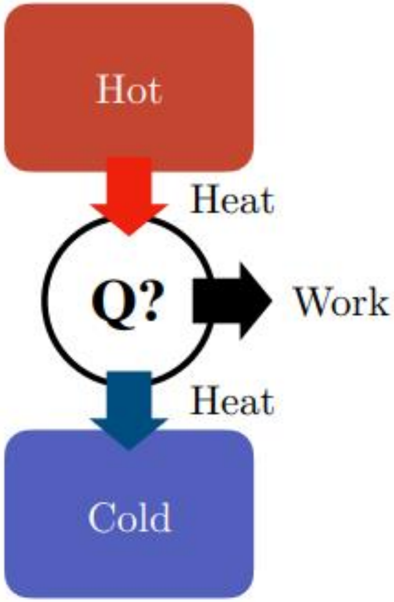

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Macroscopic thermodynamics: phenomenological theory describing the *average* behavior of heat, work and entropy.

Quantum thermodynamics: extends 'classical' concepts of heat and work into the microscopic domain.

- Thermal machines.
- Thermalization.
- Stochastic thermodynamics (fluctuations).

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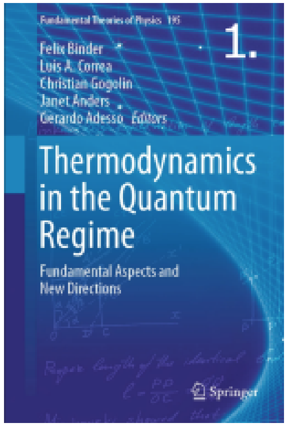
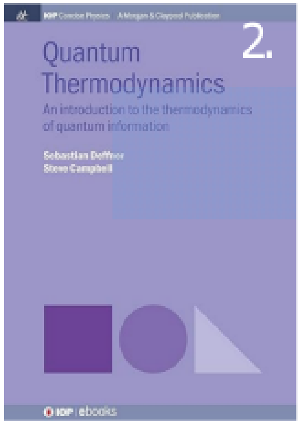
Useful literature:



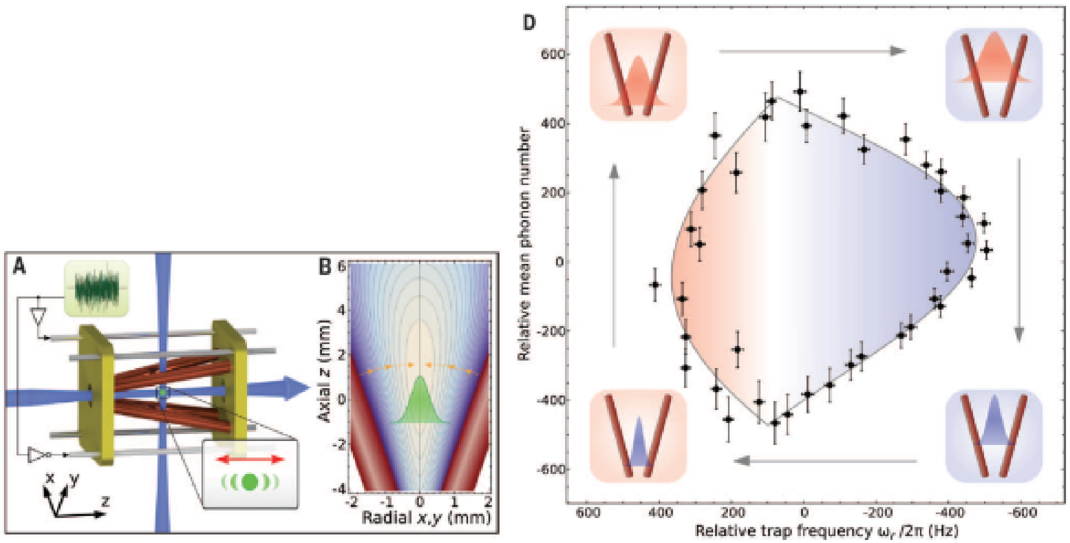


3. S. Vinjanampathy. & J. Anders, *Quantum thermodynamics*, Contemp. Phys, **57**, 545, (2016)

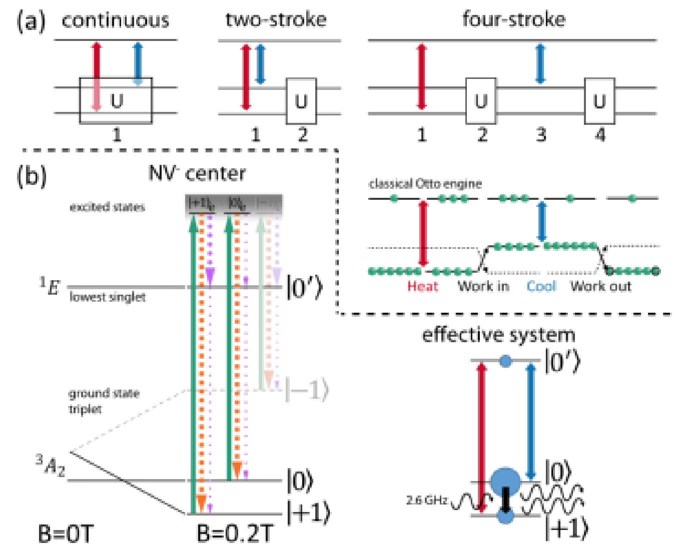
4. P. Potts, *Introduction to Quantum Thermodynamics*, arXiv:1906.07439 (2019)

Background

Technological applications:



(Roßnagel et al., Science **352**, 325-329, 2016)



(Klatzow et al., PRL, **122**, 110601, 2019)

Powering an Engine with Quantum Coherence

Janet Anders

Department of Physics and Astronomy, University of Exeter, Exeter, United Kingdom

March 20, 2019 • *Physics* 12, 32

Contents – lecture 1

Preliminaries

Quantum states

State ψ of a Isolated quantum system represented by $|\psi\rangle \in \mathcal{H}$:

$$\mathcal{H} = \{|\psi\rangle = \begin{pmatrix} c_0 \\ \vdots \\ c_{d-1} \end{pmatrix} | c_i \in \mathbb{C}\}$$

Inner (scalar) product of $\phi, \psi \in \mathcal{H}$:

$$\langle\phi|\psi\rangle = \sum_k b_k^* c_k, \qquad \langle\phi| = (b_0^*, \cdots, b_{d-1}^*),$$

with $\langle\phi| \in \mathcal{H}^*$.

D. Lidar, arXiv:1902.00967, H.-P Breuer, F. Petruccione, *The theory of open quantum systems*, 2002

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with $\langle\phi| \in \mathcal{H}^*$.

Normalization of states:

$$\||\psi\rangle\|^2 := \langle\psi|\psi\rangle = 1 \quad \Longrightarrow \quad |\psi\rangle \sim e^{i\theta}|\psi\rangle$$

Orthonormal basis $\{|k\rangle\}_{k=0}^{d-1}$ on $\mathcal{H} = \mathbb{C}^d$:

$$\langle k|k'\rangle = \delta_{kk'} \implies |\psi\rangle = \sum_k c_k |k\rangle$$

D. Lidar, arXiv:1902.00967, H.-P Breuer, F. Petruccione, *The theory of open quantum systems*, 2002

Preliminaries

Schrödinger equation

Time evolution is governed by the unitary operator $U(t) : \mathcal{H} \to \mathcal{H}$:

$$\frac{d}{dt}|\psi(t)\rangle = -\frac{i}{\hbar}H|\psi(t)\rangle \quad \Longleftrightarrow \quad |\psi(t)\rangle = U(t)|\psi(0)\rangle, \qquad t \geq 0,$$

where $H = H^\dagger$ is the Hamiltonian of the system.

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Unitary property $U^\dagger(t)U(t) = U(t)U^\dagger(t) = \mathbb{1}$.

- Conservation of probability $\|U(t)\psi\|^2 = \|\psi\|^2$.
- Spectral theorem implies $U(t) = e^{-iHt/\hbar}$ (next slide).

D. Lidar, arXiv:1902.00967, H.-P Breuer, F. Petruccione, *The theory of open quantum systems*, 2002

Preliminaries

Spectral Theorem

Any normal operator $A : \mathcal{H} \to \mathcal{H}$ satisfying $A^\dagger A = AA^\dagger$ is diagonal with respect to some orthonormal basis $\{|a\rangle\}$:

$$A = \sum_{a \in \sigma(a)} a|a\rangle\langle a| \quad \Longrightarrow \quad A|a\rangle = a|a\rangle,$$

where $\sigma(a)$ is the finite set of eigenvalues of A.

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- Observables are represented by self-adjoint operators $A = A^\dagger$, $a \in \mathbb{R}$.
- Hamiltonian $H = \sum_k E_k |k\rangle\langle k|$, with E_k the corresponding energies.

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If $f : \mathbb{C} \to \mathbb{C}$ is an analytic function:

$$f(A) = \sum_a f(a)|a\rangle\langle a| \quad \Longrightarrow \quad U(t) = \sum_k e^{-iE_k t/\hbar}|k\rangle\langle k|$$

D. Lidar, arXiv:1902.00967, H.-P Breuer, F. Petruccione, *The theory of open quantum systems*, 2002

Preliminaries

Projective measurements: For observable $A = \sum_a a|a\rangle\langle a|$, probability of measuring a is $p_a = |\langle a|\psi\rangle|^2$.

Expectation value $\langle A \rangle$:

$$\langle A \rangle = \sum_a a p_a = \sum_a a\langle a|\psi\rangle\langle\psi|a\rangle = \mathrm{Tr}(A|\psi\rangle\langle\psi|)$$

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Density matrix ρ

Pure state ensemble $\{p_{\psi_j}, |\psi_j\rangle\}$:

$$\langle A\rangle = \sum_a \sum_j a p_a p_{\psi_j} = \mathrm{Tr}(A \sum_j p_{\psi_j} |\psi_j\rangle\langle\psi_j|),$$

where $\rho = \sum_j p_{\psi_j} |\psi_j\rangle\langle\psi_j|$ is the density matrix.

Properties:

- Unit trace: $\mathrm{Tr}(\rho) = 1$.
- Hermitian: $\rho = \rho^\dagger$.
- Positive: $\langle\phi|\rho|\phi\rangle \geq 0, \quad \forall\phi \in \mathcal{H}$.

Dynamics

Liouville-von Neumann equation

Time evolution (Schrödinger equation):

$$\frac{d}{dt}\rho(t) = -i[H(t), \rho(t)] \quad \Longleftrightarrow \quad \rho(t) = U(t)\rho U^{\dagger}(t), \qquad t \geq 0,$$

where $U(t) = \mathcal{T} e^{-i\int_0^t ds\, H(s)}$ for time dependent $H(t)$.

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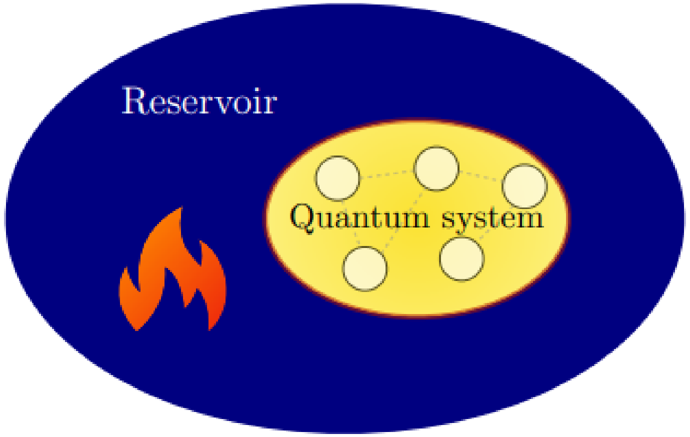
Derivation:

$$\begin{aligned}\frac{d}{dt}\rho(t) &= \left(\frac{d}{dt}U(t)\right)\rho U^\dagger(t) + U(t)\rho\left(\frac{d}{dt}U^\dagger(t)\right) \\ &= -\frac{i}{\hbar}H(t)\rho(t) + \frac{i}{\hbar}\rho(t)H(t) \\ &= -i[H(t), \rho(t)]\end{aligned}$$

D. Lidar, arXiv:1902.00967, H.-P Breuer, F. Petruccione, *The theory of open quantum systems*, 2002

Open setting

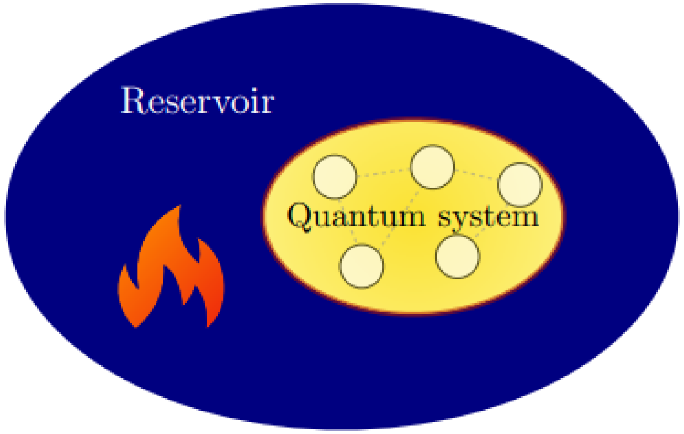
Open system S and reservoir R:



Open setting

Open system S and reservoir R:

$$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_R$$



For orthonormal bases $\{|k\rangle_S\}$ and $\{|\mu\rangle_R\}$:

$$|\psi\rangle = \sum_{k,\mu} c_{k,\mu} |k\rangle_S \otimes |\mu\rangle_R, \quad \mathcal{H} = \text{span}\{|k\rangle_S \otimes |\mu\rangle_R\}$$

Density matrix:

$$\rho = \sum_a \sum_{j,k} \sum_{\mu,\nu} p_{\psi_a} c_{a,j\mu} c^*_{a,k\nu} |j\rangle\langle k|_S \otimes |\mu\rangle\langle\nu|_R$$

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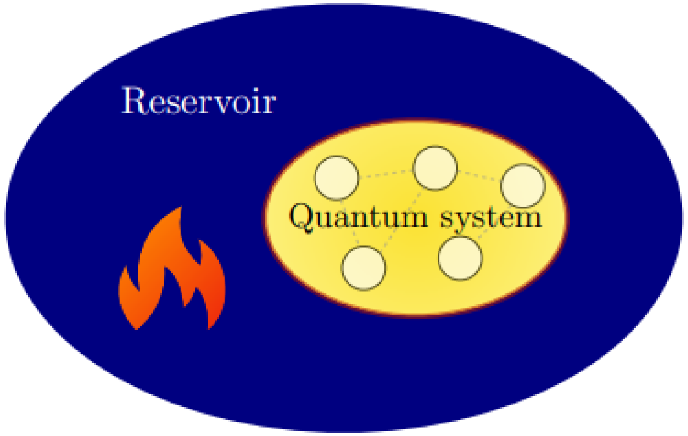

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Reduced density matrix

Expectation value:

$$\langle A_S \otimes \mathbb{1}_R \rangle = \text{Tr}_S[(A_S \otimes \mathbb{1}_R)\text{Tr}_R(\rho)] = \text{Tr}(A_S \rho_S),$$

where $\rho_S = \text{Tr}_R(\rho) = \sum_\mu \langle\mu|\rho|\mu\rangle_R$ is the reduced system density matrix.

Open setting

Time evolution of open system S:

$$\rho_S(t) = \text{Tr}_R \left(U(t)\rho(0)U^\dagger(t) \right)$$

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Time evolution of open system S:

$$\rho_S(t) = \mathrm{Tr}_R \left(U(t)\rho(0)U^\dagger(t) \right)$$

Separable $\rho = \rho_S \otimes \rho_R$:

$$\rho_S(t) = \sum_\mu \langle \mu | U(t) \rho_S \otimes \sum_\nu \lambda_\nu |\nu\rangle\langle\nu| U^\dagger(t) |\mu\rangle$$

$$= \sum_{\mu,\nu} \sqrt{\lambda_\nu} \langle \mu | U(t) | \nu \rangle \rho_S \sqrt{\lambda_\nu} \langle \nu | U^\dagger(t) | \mu \rangle = \sum_{\mu,\nu} K_{\mu\nu}(t) \rho_S(0) K^\dagger_{\mu\nu}(t)$$

Open setting

Time evolution of open system S:

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Kraus representation

The time evolution of an open quantum system under the separability condition can be described by a quantum map $\Phi_t : \mathcal{S}(\mathcal{H}_S) \to \mathcal{S}(\mathcal{H}_S)$ in Kraus form:

$$\rho_S(t) = \Phi_t \rho_S(0) = \sum_{\alpha=1}^{d^2} K_\alpha(t) \rho_S(0) K^\dagger_\alpha(t)$$

where $\sum_\alpha K^\dagger_\alpha K_\alpha = \mathbb{1}_S$.

K. Kraus, vol. **190** of Springer Lecture Notes in Physics. Springer-Verlag, Berlin, 1983

Equilibrium quantities

Von Neumann entropy of state ρ:

$$S(\rho) = -k_B \text{Tr}(\rho \ln \rho) = -k_B \sum_a \lambda_a \ln \lambda_a \geq 0$$

from the spectral decomposition $\rho = \sum_a \lambda_a |a\rangle\langle a|$.

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Gibbs state

Maximization of entropy:

$$S(\rho) = -k_B \text{Tr}(\rho \ln \rho) \leq -k_B \text{Tr}(\rho \ln \rho_G) = S_G \quad \Longrightarrow S(\rho) \leq S(\rho_G)$$

where

$$\rho_G = \frac{e^{-\beta H}}{Z}, \quad \beta = \frac{1}{k_B T}, \quad Z = \text{Tr} e^{-\beta H}$$

Gibbs state equivalent to canonical ensemble.

Relative entropy:

$$S(\rho \| \sigma) = \text{Tr}(\rho \ln \rho) - \text{Tr}(\rho \ln \sigma) \geq 0$$

Overview

In this lecture we have:

- Introduced quantum thermodynamics as an extension of macroscopic thermodynamics to the microscopic domain.
- Reviewed concepts of quantum probability and statistics.
- Formulated the time evolution of open quantum systems in terms of quantum maps.
- Reviewed equilbrium concepts.

Next lecture:

- Markovian master equations.
- 1st and 2nd laws of thermodynamics.

Thank you

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