Introduction to quantum thermodynamics

An open systems perspective

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14 Feb, 2024

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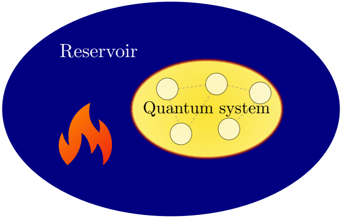

Open quantum systems:

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

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

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

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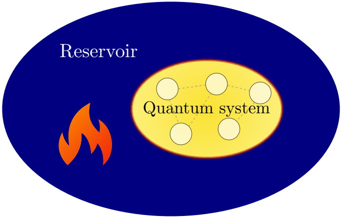

Reduced density matrix

Defined through partial trace operation $\mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H}_S)$:

$$\rho_S = \mathrm{Tr}_R(\rho) \equiv \sum_\mu \langle\mu|\rho|\mu\rangle_R$$

such that

$$\rho_S = \sum_a \sum_\mu \sum_{j,k} p_{\psi_a} c_{a,j\mu} c^*_{a,k\mu} |j\rangle\langle k|_S = \sum_{j,k} \bar{\lambda}_{jk} |j\rangle\langle k|_S$$

$\mathrm{Tr}(\rho) = 1 \implies \mathrm{Tr}_S(\rho_S) = 1.$

Encodes all measurable information about the open system S.

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

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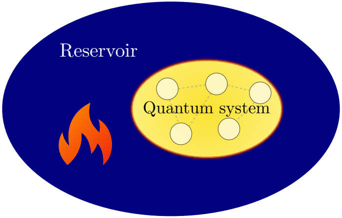

Kraus representation

Time evolution of an open system:

$$\rho_S(t) = \mathrm{Tr}_R\left(U(t)\rho(0)U^\dagger(t)\right) = \sum_{\mu,\nu} K_{\mu\nu}(t)\rho_S(0)K^\dagger_{\mu\nu}(t)$$

where $K_{\mu\nu}(t) = \sqrt{\lambda_\nu}\langle\mu|U(t)|\nu\rangle$ are Kraus operators, and $\rho_R = \sum_\nu \lambda_\nu |\nu\rangle\langle\nu|_R$.

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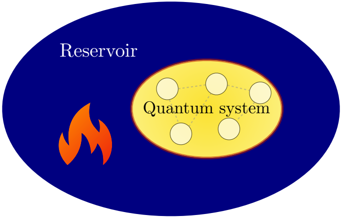

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where $K_{\mu\nu}(t) = \sqrt{\lambda_\nu}\langle\mu|U(t)|\nu\rangle$ are Kraus operators, and $\rho_R = \sum_\nu \lambda_\nu |\nu\rangle\langle\nu|_R$.

- Separability: $\rho(0) = \rho_S \otimes \rho_R$.
- Trace preservation: $\sum_{\mu,\nu} K^\dagger_{\mu\nu}K_{\mu\nu} = \mathbb{1}_S$.

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

Contents – lecture 2

Open system dynamics

Time evolution of open systems can be described in terms of a dynamical map between states:

$$\boxed{\Phi_t : \quad \mathcal{S}(\mathcal{H}_S) \rightarrow \mathcal{S}(\mathcal{H}_S)} \qquad t \geq 0$$

- Unitary operator $U(t) : |\psi(0)\rangle \rightarrow |\psi(t)\rangle$
- Dynamical map $\Phi_t : \rho(0) \rightarrow \rho(t)$

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Dynamical map

Required properties of map:

- Trace preserving: $\mathrm{Tr}[\Phi(\rho)] = \mathrm{Tr}[\rho]$
- Hermiticity: $\Phi(\rho^\dagger) = \Phi(\rho)^\dagger$
- Complete positivity: $(\Phi \otimes \mathcal{I}_A^{(k)})(\rho) \geq 0 \quad \forall k \leq d$

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Positivity corresponds to $k = 1$: $\quad \Phi(\rho) \geq 0$

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

Open system dynamics

Dynamical map

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Kraus theorem (Completely positive trace-preserving maps)

Given a linear completely positive trace-preserving (CPTP) map Φ, there exists a set of Kraus operators $K_\alpha \in \mathcal{B}(\mathcal{H}_S)$ such that

$$\Phi(\rho) = \sum_{\alpha=1}^{d^2} K_\alpha \rho K_\alpha^\dagger,$$

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

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

Semigroup

Open system dynamics can in general be described by a family of one-parameter CPTP maps $\{\Phi_t | t \geq 0, \Phi_0 = \mathcal{I}_S\}$.

Dynamical semigroup

Definition:

$$\Phi_{t+s} = \Phi_t \circ \Phi_s \qquad \forall t, s \geq 0.$$

Quantum analogue to Chapman-Kolmogorov equation.

H.-P Breuer, F. Petruccione, *The theory of open quantum systems*, 2002

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- Under certain conditions can write

$$\Phi_t = e^{\mathcal{L}t}$$

where $\mathcal{L} = \lim_{\epsilon \to 0}(\Phi_\epsilon - \mathcal{I}_S)/\epsilon$ is the corresponding generator of the map.

- Differential form:

$$\frac{d}{dt}\rho_S(t) = \left(\frac{d}{dt}\Phi_t\right)\rho_S(0) = \mathcal{L}\rho_S(t)$$

H.-P Breuer, F. Petruccione, *The theory of open quantum systems*, 2002

Semigroup

Most general form of generator $\mathcal{L}$ for quantum dynamical semigroup $\Phi_t = e^{\mathcal{L}t}$:

GKSL theorem

Markovian master equation:

$$\mathcal{L}(\rho_S) = -i[H_0, \rho_S] + \sum_{k=1}^{d^2-1} \gamma_k \left(V_k \rho_S V_k^\dagger - \frac{1}{2}\{V_k^\dagger V_k, \rho_S\} \right)$$

where

- Rates: $\gamma_k \geq 0$.
- Lindblad operators: $V_k \in \mathcal{B}(\mathcal{H}_S)$.
- Hamiltonian: $H_0 = H_0^\dagger$.

(Gorini et al., J. Math. Phys, 1976; Lindblad, Comm. Math. Phys., 1976)

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Example (Two-level system)

For $\mathcal{H}_S = \mathrm{span}\{|0\rangle, |1\rangle\}$, define $\sigma_z = |1\rangle\langle 1| - |0\rangle\langle 0|$ and $\sigma_- = \sigma_+^\dagger = |0\rangle\langle 1|$:

$$\frac{d}{dt}\rho_S = -i\frac{\omega_0}{2}[\sigma_z, \rho_S] + \gamma\left(\sigma_- \rho_S \sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho_S\}\right)$$

with ω_0 the energy difference between $|0\rangle$ and $|1\rangle$.

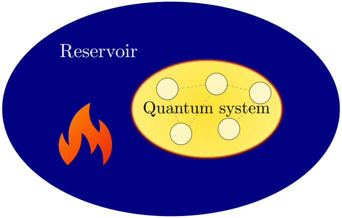
(Gorini et al., J. Math. Phys, 1976; Lindblad, Comm. Math. Phys., 1976)

System + reservoir

Total Hamiltonian:

$$H = H_S + H_R + \alpha \sum_k A_k \otimes B_k$$

where A_k and B_k are self-adjoint operators of the system and reservoir.



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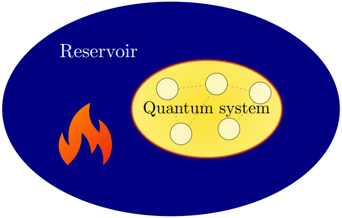

Derive Markovian master equation for $\rho_S(t) = \mathrm{Tr}_R(e^{-iHt}\rho_S(0) \otimes \pi_R(\beta)e^{iHt})$:

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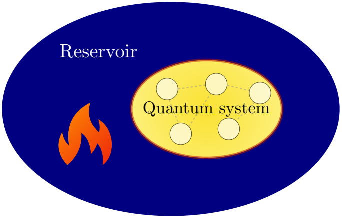


Derive Markovian master equation for $\rho_S(t) = \mathrm{Tr}_R(e^{-iHt}\rho_S(0) \otimes \pi_R(\beta) e^{iHt})$:

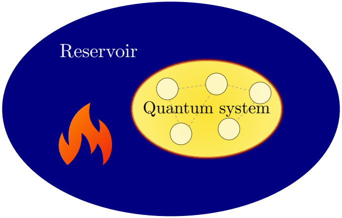
- Weak coupling $\alpha \ll 1$ (Born approximation):

$$\boxed{\rho(t) \approx \rho_S(t) \otimes \pi_R(\beta)}$$

- Thermal state of reservoir:

$$\pi_R(\beta) \equiv \frac{e^{-\beta H_R}}{Z_R}, \qquad \beta = \frac{1}{k_B T}, \qquad Z_R = \mathrm{Tr}_R\, e^{-\beta H_R}$$

System + reservoir



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- System + reservoir energy:

$$\mathrm{Tr}_R[B_k \pi_R(\beta)] = 0, \quad \forall k \implies \langle H(t) \rangle \approx \langle H_S(t) \rangle + \langle H_R \rangle_\beta$$

System + reservoir

Liouville-von Neumann equation (interaction picture):

$$\frac{d}{dt}\tilde{\rho}(t) = -i\alpha[\tilde{V}(t), \tilde{\rho}(t)] \quad \Longrightarrow \quad \tilde{\rho}(t) = \rho(0) - i\alpha \int_0^t ds\, [\tilde{V}(s), \tilde{\rho}(s)].$$

where $\tilde{V}(t) = \sum_k \tilde{A}_k(t) \otimes \tilde{B}_k(t)$.

H.-P Breuer, F. Petruccione, *The theory of open quantum systems*, 2002

System + reservoir

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where $\tilde{V}(t) = \sum_k \tilde{A}_k(t) \otimes \tilde{B}_k(t)$.

Partial trace:

$$\boxed{\frac{d}{dt}\tilde{\rho}_S(t) = -\alpha^2 \int_0^t ds\, \mathrm{Tr}_R\big[\tilde{V}(t), [\tilde{V}(t-s), \tilde{\rho}_S(t-s) \otimes \pi_R(\beta)]\big]}$$

having used $\mathrm{Tr}_R[B_k \pi_R(\beta)] = 0, \;\; \forall k.$

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Markov approximations

Partial trace:

$$\frac{d}{dt}\tilde{\rho}_S(t) = -\alpha^2 \int_0^t ds\, \mathrm{Tr}_R\big[\tilde{V}(t), [\tilde{V}(t-s), \tilde{\rho}_S(t-s) \otimes \pi_R(\beta)]\big]$$

having used $\mathrm{Tr}_R[B_k \pi_R(\beta)] = 0, \ \forall k$.

Markovian master equation (non-GKSL form)

Let τ_I and τ_R denote the interaction and reservoir time scales.

If $\tau_R \ll \tau_I$, then

$$\frac{d}{dt}\tilde{\rho}_S(t) = -\alpha^2 \int_0^\infty ds\, \mathrm{Tr}_R\big[\tilde{V}(t), [\tilde{V}(t-s), \tilde{\rho}_S(t) \otimes \pi_R(\beta)]\big].$$

Markov approximations:

1. $\int_0^t ds \to \int_0^\infty ds$: fast decaying integrand.
2. $\tilde{\rho}_S(s) \to \tilde{\rho}_S(t)$: memoryless.

H.-P Breuer, F. Petruccione, *The theory of open quantum systems*, 2002

Markov approximations

Substitute in

$$\tilde{V}(t) = \sum_k e^{-i\omega t} A_k(\omega) \otimes \tilde{B}_k(t) = \sum_k e^{i\omega t} A_k^\dagger(\omega) \otimes \tilde{B}_k(t)$$

to obtain

$$\boxed{\frac{d}{dt}\tilde{\rho}_S(t) = \alpha^2 \sum_{\omega,\omega'} \sum_{k,l} e^{i(\omega'-\omega)t} \gamma_{kl}(\omega) \Big[A_l(\omega)\tilde{\rho}_S(t) A_k^\dagger(\omega') - A_k^\dagger(\omega') A_l(\omega) \tilde{\rho}_S(t) \Big] + \text{h.c.}}$$

where

- Eigenoperators $[H_S, A_k(\omega)] = -\omega A_k(\omega)$:

$$\tilde{A}_k(t) = \sum_\omega A_k(\omega) e^{-i\omega t}$$

- Correlation functions $C_{kl}(t) = \langle \tilde{B}_k(t) B_l \rangle_\beta$:

$$\gamma_{kl}(\omega) = 2\mathrm{Re} \int_0^\infty dt\, C_{kl}(t) e^{i\omega t}$$

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Neglected Lamb shift term $S_{kl}(\omega) = \text{Im} \int_0^\infty dt\, C_{kl}(t) e^{i\omega t} \approx 0.$

H.-P Breuer, F. Petruccione, *The theory of open quantum systems*, 2002

Secular approximation

From

$$\frac{d}{dt}\tilde{\rho}_S(t) = \alpha^2 \sum_{\omega,\omega'} \sum_{k,l} e^{i(\omega'-\omega)t}\gamma_{kl}(\omega)\Big[A_l(\omega)\tilde{\rho}_S(t)A_k^\dagger(\omega') - A_k^\dagger(\omega')A_l(\omega)\tilde{\rho}_S(t)\Big] + \text{h.c.}$$

neglect off-diagonal terms $\omega \neq \omega'$:

Markovian master equation (GKSL form)

Let τ_S denote the system time scale. If $\tau_S \ll \tau_I$, then

$$\frac{d}{dt}\rho_S(t) = -i[H_S, \rho_S] + \alpha^2 \sum_{\omega} \sum_{k,l} \gamma_{kl}(\omega)\Big[A_l(\omega)\rho_S A_k^\dagger(\omega) - \frac{1}{2}\{A_k^\dagger(\omega)A_l(\omega)\}\Big]$$

where $\gamma(\omega) \geq 0$.

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where $\boldsymbol{\gamma}(\omega) \geq 0$.

Summary of approximations:

- Born (weak coupling): $\rho(t) \approx \rho_S(t) \otimes \pi_R(\beta)$
- Markov (system-reservoir time scales): $\tau_R \ll \tau_I$
- Secular (system time scales): $\tau_S \ll \tau_I$

H.-P Breuer, F. Petruccione, *The theory of open quantum systems*, 2002

Steady state

Markovian master equation (GKSL form)

$$\frac{d}{dt}\rho_S(t) = -i[H_S, \rho_S] + \alpha^2 \sum_\omega \sum_{k,l} \gamma_{kl}(\omega)\left[A_l(\omega)\rho_S A_k^\dagger(\omega) - \frac{1}{2}\{A_k^\dagger(\omega)A_l(\omega)\}\right]$$

Kubo-Martin-Schwinger (KMS) condition:

$$\langle \tilde{B}_k(-t)B_l\rangle_\beta = \langle B_l\tilde{B}_k(t-i\beta)\rangle_\beta$$

$\implies \mathcal{L}(\pi_S^\beta) = 0$, where

$$\pi_S^\beta = \frac{e^{-\beta H_S}}{Z_S}, \qquad Z_S = \text{Tr}_S e^{-\beta H_S}$$

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$\implies \mathcal{L}(\pi_S^\beta) = 0$, where

$$\pi_S^\beta = \frac{e^{-\beta H_S}}{Z_S}, \qquad Z_S = \text{Tr}_S e^{-\beta H_S}$$

is a unique stationary state of the map Φ_t, i.e. $\rho_S(t) \to \pi_S^\beta$ as $t \to \infty$.

H.-P Breuer, F. Petruccione, *The theory of open quantum systems*, 2002

1st law

System & thermal reservoir: $H(\lambda_t) = H_S(\lambda_t) + H_R + V$

- Internal energy $U(t) = \text{Tr}[H(\lambda_t)\rho(t)]$
- Von Neumann equation $\dot{\rho}(t) = -i[H(\lambda_t), \rho(t)]$

$\Delta U = W + Q$ (Vinjanampathy & Anders, CP 2016)

$$\Delta U = \int_0^t ds\, \text{Tr}[\dot{H}_S(\lambda_s)\rho_S(s)] \equiv W$$

- Weak coupling: $\text{Tr}[H(\lambda_t)\rho(t)] \approx \text{Tr}[H_S(\lambda_t)\rho_S(t)] + \text{Tr}[H_R\rho_R(t)]$

$$\Rightarrow \boxed{U_S(t) \approx \text{Tr}[H_S(\lambda_t)\rho_S(t)]}$$

- Heat: $Q = \int_0^t ds\, \text{Tr}[H_S(\lambda_s)\dot{\rho}_S(s)]$

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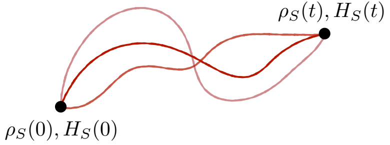

2nd law

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- Internal energy $U(t) = \text{Tr}[H(\lambda_t)\rho(t)]$
- Von Neumann equation $\dot{\rho}(t) = -i[H(\lambda_t), \rho(t)]$

$\sigma_S \geq 0$ (Vinjanampathy & Anders, CP 2016)

$$Q = \int_0^t ds\, \text{Tr}[H_S(\lambda_s)\dot{\rho}_S(s)] = \int_0^t ds\, \text{Tr}[H_S(\lambda_s)\mathcal{L}(\rho_S)]$$

- Monotonicity of relative entropy: $S(\rho_S||\pi_S^\beta) = \text{Tr}[\rho_S(\ln \rho_S - \ln \pi_S^\beta)] \geq 0$

  $S(\Phi\rho_1||\Phi\rho_2) \leq S(\rho_1||\rho_2)$

$$\mathcal{L}(\pi_S^\beta) = 0 \Rightarrow \boxed{\sigma_S \equiv -\frac{d}{dt}S(\rho_S||\pi_S^\beta) \geq 0}$$

2nd law

System & thermal reservoir: $H(\lambda_t) = H_S(\lambda_t) + H_R + V$

- Internal energy $U(t) = \text{Tr}[H(\lambda_t)\rho(t)]$
- Von Neumann equation $\dot{\rho}(t) = -i[H(\lambda_t), \rho(t)]$

$\sigma_S \geq 0$ (Vinjanampathy & Anders, CP 2016)

$$Q = \int_0^t ds\, \text{Tr}[H_S(\lambda_s)\dot{\rho}_S(s)] = \int_0^t ds\, \text{Tr}[H_S(\lambda_s)\mathcal{L}(\rho_S)]$$

- Monotonicity of relative entropy: $S(\rho_S||\pi_S^\beta) = \text{Tr}[\rho_S(\ln\rho_S - \ln\pi_S^\beta)] \geq 0$

  $S(\Phi\rho_1||\Phi\rho_2) \leq S(\rho_1||\rho_2)$

$$\mathcal{L}(\pi_S^\beta) = 0 \Rightarrow \boxed{\sigma_S \equiv -\frac{d}{dt}S(\rho_S||\pi_S^\beta) \geq 0}$$

- Spohn's inequality: $-\text{Tr}[\mathcal{L}(\rho_S)(\ln\rho_S(t) - \ln\pi_S^\beta)] \geq 0$

$$\boxed{\sigma_S = \frac{d}{dt}S(\rho_S) - \beta\dot{Q} \geq 0}$$

where $S(\rho_S) = -\text{Tr}[\rho_S \ln\rho_S]$ is the von Neumann entropy.

Overview

In this lecture we have:

- Formalized open system dynamics in terms of CPTP maps.
- For CPTP maps obeying the semigroup property, introduced the Markovian master equation (GKSL form).
- Outlined the microscopic derivation of Markovian master equations.
- Derived 1st and 2nd laws within the framework of Markovian master equations.

Next lecture:

- Applications to thermal machines (quantum Otto cycle).

Thank you

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