

Open Quantum Systems

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Summer School
on

New Directions in Quantum and Quantum Reservoir Computing,
Quantum Devices and Related Technologies

Aalto university - 18.–22.8.2025

Lecture I

Algebraic Derivation of Quantum Master Equations

- Maps that preserve state operators.
- Differential expression of the evolution law:
 - completely positive master equation (CPME)**
(AKA Lindblad-Gorini-Kossakowski-Sudarshan AKA “Markovian”).
 - (completely) bounded master equation (CBME)**
(AKA “non-Markovian” AKA Nakjima-Zwanzig).

General references for lecture I

- Bengtsson and Życzkowski, *Geometry of Quantum States. An Introduction to Quantum Entanglement*, Cambridge University Press, (2006).
- Hall et al., *Physical Review A* **89**, p. 042120, (2014). arXiv: 1009.0845
- Chruściński, *Physics Reports* **992**, pp. 1–85, (2022). arXiv: 2209.14902
- Nielsen and Chuang, *Quantum Computation and Quantum Information*, 2010 ch 8

Lecture II

II - Derivation of Quantum Master Equations from Microscopic Unitary Dynamics

- Example of exact quantum master equation: it's CB!!!
- Nakajima-Zwanzig projection method (conceptual).
- Weak coupling scaling limit.

General reference for lecture II

- Rivas and Huelga, *Open Quantum Systems*, Springer Berlin Heidelberg, (2012).

Lecture III

III - Quantum Trajectories: Stochastic Processes in a System's Hilbert Space

- Stochastic evolution of the state vector in the Hilbert space: why?
- Recovery of the completely positive master equation.
- Recovery of the completely bounded master equation.

General references for lecture III

- Carmichael, *An open systems approach to quantum optics: lectures presented at the Université libre de Bruxelles, October 28 to November 4, 1991*, Springer, (1993).
- Percival, *Quantum State Diffusion*, Cambridge University Press, (2003).
- Barchielli and Gregoratti, *Quantum Trajectories and Measurements in Continuous Time*, Springer, (2009).

Comprehensive references

- Breuer and Petruccione, *The Theory of Open Quantum Systems*, Oxford University Press, (2002).
- Wiseman and Milburn, *Quantum Measurement and Control*, Cambridge University Press, (2009).
- Jacobs, *Quantum Measurement Theory and its Applications*, Cambridge University Press, (2014).
- Lidar, “Lecture Notes on the Theory of Open Quantum Systems”, (2019). arXiv: 1902.00967.

Disclaimer

The list of references quoted in the lecture notes is largely incomplete, based on on-the-fly personal recollections during the process of preparing of the slides under time pressure. I apologize in advance for any omissions and any misattributions of findings.

First things first: Schrödinger's cat

*An aunt of my mother's also lived there with her husband, Alfred Kirk, and **six Angora cats**. (In later years there were said to be twenty.) In addition she had an ordinary **tomcat** who would very often come home from his nocturnal adventures in a sad state, so he was given the name **Thomas Becket** (referring to the Archbishop of Canterbury who was killed in office by order of King Henry II) – not that this meant a great deal to me then, nor was it very appropriate.*

***Erwin Schrödinger**, "Autobiographical Sketches", (1960)
reprinted in*

*Schrödinger, What is Life? With Mind and Matter and
Autobiographical Sketches, Cambridge University Press, (2013).*

Lecture I: Algebraic Derivation of Quantum Master Equations

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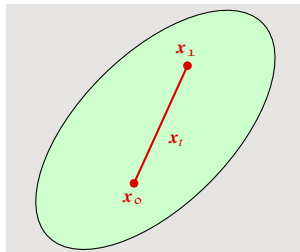
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State operators on (finite dimensional) Hilbert space \mathcal{H}

Set of state operators

$\rho \in \mathcal{M}_d(\mathbb{C})$	such that
unit trace:	$\text{Tr } \rho = 1$
self adjoint:	$\rho^\dagger = \rho$
positive eigenvalues:	$\rho \geq 0$



Stylized convex set

$$\mathcal{T}_d(\mathbb{C}) = \{\text{state operators in } \mathcal{M}_d(\mathbb{C})\} = \text{convex set}$$

Dynamical postulates for closed systems

von Neumann, *Mathematische Grundlagen der Quantenmechanik*, (1932)– English transl. (1955).

Lüders, *Annalen der Physik* **15**, pp. 663–670, (1951).

I- Unitary evolution of the state operator: Liouville-von Neumann equation

$$\begin{cases} i \partial_t \rho_t = [H, \rho_t] \\ \rho_0 = \rho_o \end{cases} \quad H = H^\dagger$$

II- Non unitary collapse of the state operator

- Experiment with \mathcal{M} distinct possible outcomes.
- To the k -th outcome we associate an operator M_k on \mathcal{H} such that

$$\sum_{k=1}^{\mathcal{M}} M_k^\dagger M_k = 1_d \quad d = \dim \mathcal{H}$$

- If we observe the k -th outcome, the state collapses to a new value

$$\rho_t \implies \rho_{t+dt} = \frac{M_k \rho(t) M_k^\dagger}{\text{Tr} \left(M_k \rho(t) M_k^\dagger \right)}$$

Similar attitudes (IMHO)

von Neumann, *Mathematische Grundlagen der Quantenmechanik*.
(English translation “*The Mathematical Foundations of Quantum Mechanics*”, Princeton University Press 1955), 1932

Kolmogorov, *Grundbegriffe der Wahrscheinlichkeitsrechnung* (English translation “*Foundations of the theory of probability*”, Chelsea Publishing Company, 1956), 1933

Define the minimum set of postulates under which a mathematical theory can be developed, putting aside their “ontological interpretation”.

Question:

What if we relinquish the unitary evolution postulate?
“*Stochastic Dynamics of Quantum-Mechanical Systems*”

Sudarshan, Mathews, and Rau, *Physical Review* **121**, pp. 920–924, (1961).

Motivation: dynamics of open quantum systems.

Mathematical problem: linear maps Φ on $\mathcal{M}_d(\mathbb{C})$

Q: Why linear maps? A: Bridge relation

$$E_P \mathcal{A} = \text{Tr}(\rho A) \implies \Phi \left(\sum_{i=1}^N x_i O_i \right) = \sum_{i=1}^N x_i \Phi(O_i) \quad x_i \in \mathbb{R}$$

Upshot: we need to understand linear maps in first place!

$\mathcal{M}_d(\mathbb{C})$ as a Hilbert space

Hilbert-Schmidt inner product

$$\langle A, B \rangle = \text{Tr} \left(A^\dagger B \right) \quad \forall A, B \in \mathcal{M}_d(\mathbb{C})$$

Canonical (computational) basis of $\mathcal{M}_d(\mathbb{C})$

$$E_{i,j} = \mathbf{e}_i \mathbf{e}_j^\dagger \quad i, j = 1, \dots, d \quad \& \quad \{\mathbf{e}_i\}_{i=1}^d \text{ computational basis of } \mathcal{H} = \mathbb{C}^d$$

$$\begin{array}{ccc} \mathcal{M}_d(\mathbb{C}) & \Leftrightarrow & \mathbb{C}^{d^2} \\ O = \sum_{i,j=1}^d E_{i,j} \text{Tr} \left(E_{i,j}^\dagger O \right) \in \mathcal{M}_d(\mathbb{C}) & \Leftrightarrow & \text{res}(O) = \sum_{i,j=1}^d \mathbf{e}_i \otimes \bar{\mathbf{e}}_j \langle \mathbf{e}_i, O \mathbf{e}_j \rangle \end{array}$$

Representation of a map in the computational basis

$$O' = \Phi(O) \quad \Leftrightarrow \quad O'_{i,j} = \sum_{m,n=1}^d \Phi_{i,j,m,n} O_{m,n} \quad \text{with } O_{i,j} = \text{Tr} \left(E_{i,j}^\dagger O \right)$$

Spectral decomposition of linear maps

Dual representation (Heisenberg picture)

$$\begin{aligned}\mathrm{Tr} \left(A^\dagger \Phi(B) \right) &= \sum_{i,j,m,n=1}^d \overline{A_{i,j}} \Phi_{i,j,m,n} B_{m,n} \\ &= \sum_{i,j,m,n=1}^d \overline{\Phi_{i,j,m,n}} A_{i,j} B_{m,n} := \mathrm{Tr} \left(\left((\Phi^\dagger(A))^\dagger B \right) \right)\end{aligned}$$

Spectral problem

$$\begin{aligned}\Phi(R^{(\ell)}) &= \ell^{(\ell)} R^{(\ell)} & \Leftrightarrow & \sum_{m,n=1}^d \Phi_{i,j,m,n} R_{m,n}^{(\ell)} = \ell^{(\ell)} R_{i,j}^{(\ell)} \\ \Phi^\dagger(L^{(\ell)}) &= \overline{\ell^{(\ell)}} L^{(\ell)} & \Leftrightarrow & \sum_{m,n=1}^d \overline{\Phi_{m,n,i,j}} L_{m,n}^{(\ell)} = \overline{\ell^{(\ell)}} L_{i,j}^{(\ell)}\end{aligned}$$

$$\Phi(O) = \sum_{\ell=0}^{d^2-1} \ell^{(\ell)} R^{(\ell)} \mathrm{Tr} (L^{(\ell) \dagger} O) \quad \text{non degenerate eigenvalues}$$

Linear maps preserving state operators

1) Φ preserves the trace: $\forall O \in \mathcal{M}_d(\mathbb{C})$

$$\text{Tr}(O) = \text{Tr}(\Phi(O)) = \text{Tr}(\Phi^\dagger(1_d) O) \implies \Phi^\dagger(1_d) = 1_d$$

2) Φ maps self-adjoint to self-adjoint: $\forall O \in \mathcal{M}_d(\mathbb{C})$

$$(\Phi(O))^\dagger = \Phi(O^\dagger) \qquad (\Phi^\dagger(O))^\dagger = \Phi^\dagger(O^\dagger)$$

3) Φ maps positive to positive: $\forall O \in \mathcal{M}_d(\mathbb{C})$

$$\text{if} \qquad O \geq 0 \qquad \text{then} \qquad \Phi(O) \geq 0$$

Jargon:

positive map = 3) holds true

The adjective thus does not refer to the spectral properties of the map itself.

Positive & trace preserving maps Φ are contractive

Kossakowski, *Reports on Mathematical Physics* **3**, 247–274, (1972).

Pérez-García et al., *Journal of Mathematical Physics* **47**, (2006). arXiv: math-ph/0601063.

Trace norm:

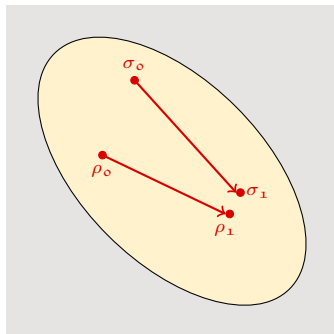
$$\|O\|_1 = \text{Tr} \sqrt{O^\dagger O} \quad \Rightarrow \quad O^\dagger = O : \|O\|_1 = \sum_{i=1}^d |\lambda_i(O)|$$

$$O = O^\dagger = O_+ - O_-$$

$$\begin{aligned} \|\Phi(O)\|_1 &= \|\Phi(O_+) - \Phi(O_-)\|_1 \\ &\leq \|\Phi(O_+)\|_1 + \|\Phi(O_-)\|_1 \\ &= \text{Tr}(\Phi(O_+)) + \text{Tr}(\Phi(O_-)) \\ &= \text{Tr}(O_+) + \text{Tr}(O_-) = \|O\|_1 \end{aligned}$$

Contraction of trace distance:

$$\|\Phi(\rho_0 - \sigma_0)\|_1 \leq \|\rho_0 - \sigma_0\|_1$$



Sz.-Nagy (Szökefalvi-Nagy) unitary dilation theorem

Let T be a contraction operator on a Hilbert space \mathcal{H} . Then there is a Hilbert space \mathcal{A} containing \mathcal{H} as a subspace and a unitary operator U on \mathcal{A} such that

$$T = P_{\mathcal{H}} U|_{\mathcal{H}}$$

$$\mathcal{H} = \mathbb{C}^d$$

$$U = \begin{bmatrix} T & -\left(1_d - T T^\dagger\right)^{1/2} \\ \left(1_d - T^\dagger T\right)^{1/2} & T^\dagger \end{bmatrix}$$

Paulsen, *Completely Bounded Maps and Operator Algebras*, Cambridge University Press, (2003).

Upshot: **positive trace preserving maps** can always be thought as the **restriction to a subsystem** of a **unitary evolution** in an embedding Hilbert space.

“Quantum” Perron-Frobenius theorem

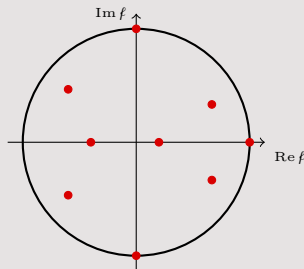
Properties of positive trace preserving maps on $\mathcal{M}_d(\mathbb{C})$

- 1 There is an eigenvalue ℓ with largest real part that is exactly equal to the unity i.e. $\ell = 1$ with eigenvector O_\star

$$\Phi(O_\star) = O_\star$$

that is a positive matrix: $O_\star \geq 0$.

- 2 All eigenvalues ℓ belong to the the unit disk of \mathbb{C} .
- 3 The spectrum is symmetric with respect to the real axis.



Idea of the proof:

A positive and trace preserving linear map sends the set of state operators into itself. The set is **convex** and **compact** and is a Banach space with respect to the trace norm: invoke **Brouwer's fixed-point theorem**

Operator sum representation of linear maps

Sudarshan's reshuffling involution:

$$(\Phi^R)_{i,j,m,n} = \Phi_{i,m,j,n}$$

Then, assuming non degeneration:

$$\begin{aligned}(\Phi^R(O))_{i,j} &= \sum_{m,n=1}^d (\Phi^R)_{i,j,m,n} O_{m,n} = \sum_{\ell=1}^{d^2} f^{(\ell)} \tilde{R}_{i,j}^{(\ell)} \sum_{m,n=1}^d \tilde{L}_{m,n}^{(\ell)} O_{m,n} \\ \Rightarrow (\Phi(O))_{i,j} &= \sum_{m,n=1}^d (\Phi^R)_{i,m,j,n} O_{m,n} = \sum_{\ell=1}^{d^2} f^{(\ell)} \sum_{m,n=1}^d \tilde{R}_{i,m}^{(\ell)} O_{m,n} \tilde{L}_{j,n}^{(\ell)}\end{aligned}$$

Upshot: a linear map in operator sum form

$$\Phi(O) = \sum_{\ell,k=1}^{d^2} c_{\ell,k} A^{(\ell)} O B^{(k)\dagger} \quad \text{for some} \quad \begin{array}{l} c_{\ell,k} \in \mathbb{C} \\ A^{(\ell)}, B^{(k)} \in \mathcal{M}_d(\mathbb{C}) \end{array} \quad \ell,k=1,\dots,d^2$$

Linear maps preserving state operators

$$\Phi(O) = \sum_{\ell,k=1}^{d^2} c_{\ell,k} A^{(\ell)} O B^{(\ell)\dagger}$$

1) Φ preserves the trace: $\forall O \in \mathcal{M}_d(\mathbb{C})$

$$\text{Tr}(O) = \text{Tr}(\Phi(O)) \quad \implies \quad \sum_{\ell,k=1}^{d^2} c_{\ell,k} B^{(\ell)\dagger} A^{(\ell)} = 1_d$$

2) Φ maps self-adjoint to self-adjoint: $\forall O \in \mathcal{M}_d(\mathbb{C})$

$$(\Phi(O))^\dagger = \Phi(O^\dagger) \quad \implies \quad \begin{aligned} c_{\ell,k} &= \bar{c}_{k,\ell} \\ B^{(\ell)} &= A^{(\ell)} \end{aligned} \quad \ell, k=1, \dots, d^2$$

3) Φ maps positive to positive: ?

A sufficient condition: complete positivity (CP)

Assume $[c_{\ell,k}]$ a positive matrix: upon diagonalizing

$$\Phi(O) = \sum_{\ell=1}^{d^2} V^{(\ell)} O V^{(\ell)\dagger} \quad (\text{Kraus positive operator sum})$$

Reshuffling & reshaping a CP map into a matrix on \mathbb{C}^{d^2}

$$\Phi^R(O) = \sum_{\ell=1}^{d^2} V^{(\ell)} \text{Tr}(V^{(\ell)\dagger} O)$$

$$\text{res}(\Phi^R(O)) = \left(\sum_{\ell=1}^{d^2} \text{res}(V^{(\ell)}) \text{res}^\dagger(V^{(\ell)}) \right) \text{res}(O)$$

Choi-Jamiołkowski : $\psi = \sum_{i=1}^d e_i \otimes e_i \in \mathbb{C}^d \otimes \mathbb{C}^d$

$$\sum_{i,j=1}^d (\Phi \otimes \text{Id})(\psi \psi^\dagger) = \sum_{\ell=1}^{d^2} \text{res}(V^{(\ell)}) \text{res}^\dagger(V^{(\ell)}) \geq 0$$

CP is only a sufficient condition

State operator if and only if $\sum_{i=1}^3 x_i^2 \leq 1$

$$\rho = \frac{1_2 + \sum_{i=1}^3 x_i \sigma_i}{2}$$

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

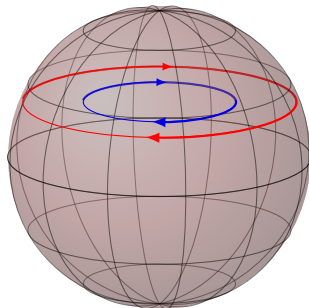
$$\sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\sigma_3 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

PTP but not CPTP map

$$\Phi(\rho) = \frac{\rho + \sum_{i=1}^2 \sigma_i \rho \sigma_i - \sigma_3 \rho \sigma_3}{2}$$

Pearle, *European Journal of Physics*
33, pp. 805–822, (2012). arXiv:
1204.2016



State operators must satisfy
 $\sum_{i=1}^3 x_i^2 \leq 1$

Physical motivation for CPTP evolution maps

Partial trace of unitary evolution on $\mathcal{H} \otimes \mathcal{H}^{(E)}$

$$\Phi_{t,0}(\rho_{\circ}) = \text{Tr}_{\mathcal{H}^{(E)}} \left(U_{t,0} \rho_{\circ}^{(E)} \otimes \rho_{\circ} U_{t,0}^{\dagger} \right) = \sum_{\ell=1}^N V_{t,0}^{(\ell)} \rho_{\circ} V_{t,0}^{(\ell)\dagger}$$

Q: is a “physical” necessarily a CPTP evolution?

Pechukas, *Physical Review Letters* **73**, pp. 1060–1062, (1994).

Alicki, *Physical Review Letters* **75**, pp. 3020–3020, (1995).

Shaji and Sudarshan, *Physics Letters A* **341**, pp. 48–54, (2005).

Dominy and Lidar, *Quantum Information Processing* **15**, pp. 1349–1360, (2015). arXiv: 1503.05342v2

the partition of a quantum system into subsystems is dictated by the set of operationally accessible interactions and measurements
Zanardi, Lidar, and Lloyd, *Physical Review Letters* **92**, (2004). arXiv: quant-ph/0308043.

Evolution law: $\forall O \in \mathcal{M}_d(\mathbb{C})$ (initial data)

Semigroup property + regularity requirements:

$$\begin{aligned}\Phi_{t,u}(\Phi_{u,s}(O)) &= \Phi_{t,s}(O) \\ \Phi_{t,t}(O) &= O\end{aligned}\quad \forall t \geq u \geq s \geq 0$$

Infinitesimal generator

$$\begin{aligned}\frac{d}{dt}\Phi_{t,s}(O) &= \lim_{\varepsilon \downarrow 0} \frac{\Phi_{t+\varepsilon,s}(O) - \Phi_{t,s}(O)}{\varepsilon} \\ &= \lim_{\varepsilon \downarrow 0} \frac{\Phi_{t+\varepsilon,t}(\Phi_{t,s}(O)) - \Phi_{t,s}(O)}{\varepsilon} \\ &= \lim_{\varepsilon \downarrow 0} \frac{\Phi_{t+\varepsilon,t} - \text{Id}}{\varepsilon} \circ (\Phi_{t,s}(O)) := \mathfrak{L}_t(\Phi_{t,s}(O))\end{aligned}$$

Semigroup of CPTP maps \implies GKLS generator

All elements are CPTP maps

$$\Phi_{t,s}(O) = \sum_{\ell=1}^N V_{t,s}^{(\ell)} O V_{t,s}^{(\ell)\dagger}$$

Infinitesimal generator in **canonical** form

Gorini, Kossakowski, and Sudarshan, *Journal of Mathematical Physics* **17**, (1976). .

Lindblad, *Communications in Mathematical Physics* **48**, (1976). .

$$\mathfrak{L}_t(O) = -i [H_t, O] + \sum_{\ell=1}^{d^2-1} c_t^{(\ell)} \left(L_t^{(\ell)} O L_t^{(\ell)\dagger} - \frac{L_t^{(\ell)\dagger} L_t^{(\ell)} O + O L_t^{(\ell)\dagger} L_t^{(\ell)}}{2} \right)$$

$$\begin{cases} c_t^{(\ell)} \geq 0 \\ \text{Tr} (L_t^{(\ell)\dagger} L_t^{(k)}) = \delta_{\ell,k} \\ \text{Tr} (L_t^{(\ell)}) = 0 \end{cases} \quad \forall t \geq 0 \quad \& \quad \forall \ell, k = 1, \dots, d^2 - 1$$

all functional dependence on time continuous and bounded

GKLS generator \implies semigroup of CPTP maps

A system of first order differential equations generates a semigroup: $\forall t \geq s$

$$\frac{d\rho_t}{dt} = -i [H_t, \rho_t] + \sum_{\ell=1}^{d^2-1} c_t^{(\ell)} \left(L_t^{(\ell)} \rho_t L_t^{(\ell)\dagger} - \frac{L_t^{(\ell)\dagger} L_t^{(\ell)} \rho_t + \rho_t L_t^{(\ell)\dagger} L_t^{(\ell)}}{2} \right)$$

$$\rho_s = \rho_0$$

Define $V_{t,s} = \mathcal{T} \exp \left(\int_s^t du \left(-i H_u + \sum_{\ell=0}^{d^2-1} L_u^{(\ell)\dagger} L_u^{(\ell)} / 2 \right) \right)$

$$\rho_t = V_{t,s} \sigma_t V_{t,s}^\dagger$$

$$\frac{d\sigma_t}{dt} = - \sum_{\ell=1}^{d^2-1} c_t^{(\ell)} \tilde{L}_{t,s}^{(\ell)} \sigma_t \tilde{L}_{t,s}^{(\ell)\dagger}$$

$$\tilde{L}_{t,s}^{(\ell)} = V_{t,s}^{-1} L_t^{(\ell)} V_{t,s}$$

The composition of CP maps is CP

Is every CPTP $\Phi_{t,0}$ solution of a GLKS master equation?

NO!!!

1 Suppose we only know

$$\Phi_{t,0}(O) = \sum_{\ell=1}^N V_{t,0}^{(\ell)} O V_{t,0}^{(\ell)\dagger} \quad \forall t \geq 0$$

$$\Rightarrow \text{res}(\Phi_{t,0}(O)) = \sum_{\ell=1}^N V_{t,0}^{(\ell)} \otimes \overline{V_{t,0}^{(\ell)}} \text{res}(O) := \mathcal{F}_t \text{res}(O)$$

2 Assume differentiability

$$\frac{d}{dt} \mathcal{F}_t \text{res}(O) = \left(\frac{d\mathcal{F}_t}{dt} \mathcal{F}_t^{-1} \right) \mathcal{F}_t \text{res}(O) := \mathcal{L}_t \mathcal{F}_t \text{res}(O)$$

3 Use that reshaping is an isomorphism $\mathcal{M}_d(\mathbb{C}) \Leftrightarrow \mathbb{C}^{d^2}$ to identify the generator \mathcal{L}_t

In other words: the CPTP family $\Phi_{t,0}$ belong to a semigroup whose generic $\Phi_{t,s}$ element is only trace and self-adjoint preserving.

Two comments:

The reshaped generator is no unicorn

Horn and Johnson, *Topics in Matrix Analysis*, Cambridge University Press, (1991).

$$\begin{aligned}\mathcal{L}_t = & -\imath \left(H_t \otimes 1_d - 1_d \otimes H_t^\top \right) \\ & + \sum_{\ell=1}^{d^2-1} c_t^{(\ell)} \left(L_t^{(\ell)} \otimes \overline{L_t^{(\ell)}} - \frac{L_t^{(\ell) \dagger} L_t^{(\ell)} \otimes 1_d + 1_d \otimes L_t^{(\ell) \top} \overline{L_t^{(\ell)}}}{2} \right)\end{aligned}$$

CP \neq CP-divisible

$$\Phi_{t,0}(O) = \Phi_{t,t_n} \circ \Phi_{t_n,t_{n-1}} \circ \cdots \circ \Phi_{t_1,0}(O) \quad t \geq t_n \geq \cdots \geq t_0 \geq 0$$

- $\Phi_{t,0}$ is CP.
- Some of the Φ_{t_{i+i},t_i} may not be.

Nakjima-Zwanzig (completely bounded) master equation

Positivity for any $t \geq s \geq 0$ **not** granted for all initial data

$$\frac{d\rho_t}{dt} = -\imath [H_t, \rho_t] + \sum_{\ell=1}^{d^2-1} c_t^{(\ell)} \left(L_t^{(\ell)} \rho_t L_t^{(\ell)\dagger} - \frac{L_t^{(\ell)\dagger} L_t^{(\ell)} \rho_t + \rho_t L_t^{(\ell)\dagger} L_t^{(\ell)}}{2} \right)$$

$$\rho_s = \rho_0 \quad s \geq 0$$

$$\begin{cases} |c_t^{(\ell)}| < \infty \\ \text{Tr} (L_t^{(\ell)\dagger} L_t^{(k)}) = \delta_{\ell,k} & \forall t \geq 0 \quad \& \quad \forall \ell, k = 1, \dots, d^2 - 1 \\ \text{Tr} (L_t^{(\ell)}) = 0 \end{cases}$$

Canonical form of the solution semigroup

Wittstock, *Journal of Functional Analysis* **40**, pp. 127–150, (1981).

Paulsen, *Proceedings of the American Mathematical Society* **86**, pp. 91–96, (1982).

$$\Phi_{t,s}(O) = \sum_{\ell=1}^{N_+} V_{t,s}^{(\ell)} O V_{t,s}^{(\ell)\dagger} - \sum_{\ell=1}^{N_-} W_{t,s}^{(\ell)} O W_{t,s}^{(\ell)\dagger} \quad N_+ + N_- = d^2$$

$$\sum_{\ell=1}^{N_+} V_{t,s}^{(\ell)\dagger} V_{t,s}^{(\ell)} - \sum_{\ell=1}^{N_-} W_{t,s}^{(\ell)\dagger} W_{t,s}^{(\ell)} = 1_d$$

Summary

- **Complete positivity** is a **sufficient condition** for a linear map to be positivity preserving (=positive map).
- **Complete positivity** naturally arises from the **partial trace** on the unitary evolution of initial conditions in **tensor product form**. From the operative point of view, one can make a strong case for adopting initial data in tensor product form in order to define the concept of subsystem in quantum mechanics.
- A **completely positive trace preserving (CPTP) map** act on the system state operator as a **generalized measurement**.
- Cornerstone result:
CPTP semigroup \Leftrightarrow GLKS (completely positive) master equation \Leftrightarrow state operators always evolve in state operator.
- There exist **CPTP differentiable maps** that are **not solution** of a completely positive master equation.

Lecture II: Derivation of Quantum Master Equations from Microscopic Unitary Dynamics

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Exactly integrable example: the Jaynes Cummings model

Jaynes and Cummings, *Proceedings of the IEEE* **51**, pp. 89–109, (1963).

Shore and Knight, *Journal of Modern Optics* **40**, pp. 1195–1238, (1993).

Babelon, “A Short Introduction to Classical and Quantum Integrable Systems” (2007).

Model of 2-level atom interaction with radiation

$$i \dot{\psi}_t = H \psi_t$$

$$H = \frac{\omega + \delta}{2} \sigma_3 + \omega a^\dagger a + g a \sigma_+ + \bar{g} a^\dagger \sigma_-$$

Under this Hamiltonian the Hilbert space

$$\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{L}^2(\mathbb{R})$$

foliates into invariant sub-spaces with n -quanta.

Initial state for the closed system

$$\psi_0 = (\cos \theta e_1 + \sin \theta e_2) \otimes \Phi_0$$

$e_1, e_2 =$ computational basis spin states
 $\Phi_0 =$ boson ground state

Exact master equation for Jaynes Cummings

Smirne and Vacchini, *Physical Review A* **82**, (2010). arXiv: 1005.1604.

Donvil and Muratore-Ginanneschi, *Open Systems & Information Dynamics* **30**, (2023). arXiv: 2309.13408.

Master equation for the qubit

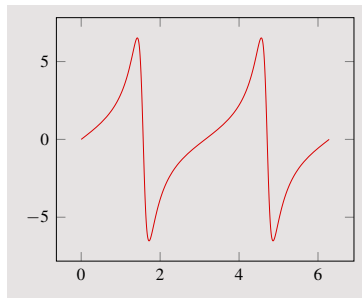
$$\dot{\rho}_t = -i \operatorname{Im} \left(\frac{\dot{\gamma}_t}{\gamma_t} \right) \left[\frac{\sigma_3}{2}, \rho_t \right] + c_t \left(\sigma_- \rho_t \sigma_+ - \frac{\sigma_+ \sigma_- \rho_t + \rho_t \sigma_+ \sigma_-}{2} \right)$$

Parameters

$$c_t = -\frac{\bar{\gamma}_t \dot{\gamma}_t + \dot{\bar{\gamma}}_t \gamma_t}{|\gamma_t|^2}$$

$$\gamma_t = e^{i(\frac{\delta}{2} + \omega)t} \left(\cos(\nu t) + \frac{i\delta}{2\nu} \sin(\nu t) \right)$$

$$\nu = \sqrt{\frac{\delta^2}{4} + \omega^2}$$



Canonical coupling c_t over one period for $\delta = 0.3$ and $\nu = 1$

General bipartite system

Liouville-von Neumann equation

$$\begin{cases} i \partial_t \rho_t = [H, \rho_t] \\ \rho_0 = \rho^{(S)} \otimes \rho^{(E)} \end{cases} \quad H = H^{(S)} \otimes 1_{\mathcal{H}^{(E)}} + 1_{\mathcal{H}^{(S)}} \otimes H^{(E)} + H^{(\iota)}$$

Assumption on the environment initial data

$$\begin{aligned} [H^{(E)}, \rho_0^{(E)}] &= 0 \\ H^{(\iota)} &= g \sum_{i=1}^N A^{(i)} \otimes B^{(i)} \quad \text{Tr} (B^{(i)} \rho_0^{(E)}) = 0 \quad \forall i = 1, \dots, N \end{aligned}$$

Dirac's interaction picture

$$\begin{cases} i \partial_t \tilde{\rho}_t = [\tilde{H}_t, \tilde{\rho}_t] \\ \tilde{\rho}_0 = \rho_0^{(S)} \otimes \rho_0^{(E)} \end{cases} \quad \text{where:} \quad \begin{aligned} \tilde{\rho}_t &= U_t^\dagger \rho_t U_t \\ \tilde{H}_t &= U_t^\dagger H^{(\iota)} U_t \\ U_t &= \exp \left(-i \left(H^{(S)} \otimes 1_{\mathcal{H}^{(E)}} + 1_{\mathcal{H}^{(S)}} \otimes H^{(E)} \right) t \right) \end{aligned}$$

Nakajima-Zwanzig projector

Rivas and Huelga, *Open Quantum Systems*, Springer Berlin Heidelberg, (2012). ch 5

Breuer and Petruccione, *The Theory of Open Quantum Systems*, Oxford University Press, (2002). ch 9

Maps operators on $\mathcal{H}^{(S)} \otimes \mathcal{H}^{(E)}$ to operators on $\mathcal{H}^{(S)} \otimes \mathcal{H}^{(E)}$

$$\mathfrak{P}(\rho_t) = (\text{Tr}_{\mathcal{H}^{(E)}} \rho_t) \otimes \rho_0^{(E)} \equiv \rho_t^{(S)} \otimes \rho_0^{(E)}$$

- $\mathfrak{P}^2(\rho_t) = \mathfrak{P}(\rho_t)$ is a projector.
- $\widetilde{\mathfrak{P}(\rho_t)} = \mathfrak{P}(\tilde{\rho}_t)$ commutes with the interaction picture map.
- $\mathfrak{P}^\perp(\rho_t) = \rho_t - \mathfrak{P}(\rho_t)$ is also projector.

Orthogonal decomposition of the state operator

$$\tilde{\rho}_t = \mathfrak{P}(\tilde{\rho}_t) + \mathfrak{P}^\perp(\tilde{\rho}_t)$$

Nakajima-Zwanzig equivalent system

Linear system for $\sigma_t = \mathfrak{P}(\tilde{\rho}_t)$ & $\sigma_t^\perp = \mathfrak{P}^\perp(\tilde{\rho}_t)$

$${}_i \partial_t \tilde{\rho}_t = [\tilde{H}_t^{(\iota)}, \tilde{\rho}_t] \implies \begin{cases} {}_i \partial_t \sigma_t = \mathfrak{P}([\tilde{H}_t^{(\iota)}, \sigma_t]) + \mathfrak{P}([\tilde{H}_t^{(\iota)}, \sigma_t^\perp]) \\ {}_i \partial_t \sigma_t^\perp = \mathfrak{P}^\perp([\tilde{H}_t^{(\iota)}, \sigma_t]) + \mathfrak{P}^\perp([\tilde{H}_t^{(\iota)}, \sigma_t^\perp]) \end{cases}$$

Strategy: solve for σ_t^\perp and obtain a closed equation for σ_t

- $\sigma_0^\perp = 0$ initial condition is a tensor product.
- $\sigma_t^\perp = -{}_i \int_0^t ds \mathfrak{P}^\perp([\tilde{H}_s^{(\iota)}, \sigma_s]) - {}_i \int_0^t ds \mathfrak{P}^\perp([\tilde{H}_s^{(\iota)}, \sigma_s^\perp])$
can be solved by infinite iteration: Born series.

$$\sigma_t^\perp = -{}_i \int_0^t ds G_{t,s} \mathfrak{P}^\perp([\tilde{H}_s^{(\iota)}, \sigma_s])$$

Integro-differential equation in $\mathcal{H} = \mathcal{H}^{(S)} \otimes \mathcal{H}^{(E)}$

$$\partial_t \sigma_t = -{}_i \mathfrak{P}([\tilde{H}_t^{(\iota)}, \sigma_t]) - \int_0^t ds \mathfrak{P}([\tilde{H}_t^{(\iota)}, G_{t,s} \mathfrak{P}^\perp([\tilde{H}_s^{(\iota)}, \sigma_s])])$$

Closed equation in $\mathcal{H}^{(S)}$

$\tilde{\rho}_t^{(S)} = \text{Tr}_{\mathcal{H}^{(E)}}(\sigma_t)$ **and using** $\text{Tr}(B^{(i)} \rho_0^{(E)}) = 0$ **for all** i

$$\partial_t \tilde{\rho}_t^{(S)} = -\text{Tr}_{\mathcal{H}^{(E)}} \left(\int_0^t ds \mathfrak{P} \left(\left[\tilde{H}_t^{(\iota)}, G_{t,s} \left[\tilde{H}_s^{(\iota)}, \tilde{\rho}_s^{(S)} \otimes \rho_0^{(E)} \right] \right] \right) \right)$$

Summary of the Nakajima-Zwanzig method

- It's not a way to solve the Liouville-von Neumann equation.
- It is of conceptual importance: it **defines** the open system dynamics.
- The kernel $G_{t,s}$ can be approximated by truncating the Born series.
- Integro-differential equation: the environment is modeled by a memory kernel.

From Nakajima-Zwanzig to master equations

Shimizu, *Journal of the Physical Society of Japan* **28**, pp. 1088–1088, (1970).

Chruściński and Kossakowski, *Physical Review Letters* **104**, p. 070406, (2010). arXiv: 0912.1259

Nestmann, Bruch, and Wegewijs, *Physical Review X* **11**, p. 021041, (2021). arXiv: 2002.07232

Reshaped integro differential equation: $r_t = \text{res}(\tilde{\rho}_t^{(s)})$

$$\partial_t r_t = \int_0^t ds \mathcal{K}_{t,s} r_s$$

We would like to find \mathcal{L}_t such that

$$\partial_t r_t = \mathcal{L}_t r_t \quad \implies \quad r_t = \mathcal{F}_{t,0} r_0 = \mathcal{T} \exp \left(\int_0^t ds \mathcal{L}_s \right) r_0$$

Fixed point equation: “time-convolutionless” P.T.

$$\left\{ \begin{array}{l} \partial_t \mathcal{F}_{t,s} = \mathcal{L}_t \mathcal{F}_{t,s} \\ \partial_t \mathcal{F}_{s,t} = -\mathcal{F}_{s,t} \mathcal{L}_t \end{array} \right. \implies \mathcal{L}_t = \int_0^t ds \mathcal{K}_{t,s} \mathcal{A} \exp \left(- \int_s^t ds \mathcal{L}_s \right)$$

Where did all our memories go?

van Wonderen and Lendi, *Journal of Statistical Physics* **100**, pp. 633–658, (2000).

Chruściński and Kossakowski, *Physical Review Letters* **104**, p. 070406, (2010). arXiv: 0912.1259

- The master equation **depends** on the time t_ℓ ($=0$ for convenience) when

$$\rho_{t_\ell} = \rho_{t_\ell}^{(S)} \otimes \rho_{t_\ell}^{(E)}$$

- The fixed point equation is equivalent to find the inverse of an integral kernel. In general, we expect this to be possible only **locally**.
- Physical consequence: we expect master equations to be **generically** accurate only on **finite time intervals**.

The van Hove scaling limit (vHSL): preparation

van Hove, *Physica* **21**, 517–54, (1954).

Davies, *Communications in Mathematical Physics* **39**, pp. 91–110, (1974).

Assumptions on the system's spectrum (possible to milden)

- We suppose the spectrum non degenerate

$$\epsilon_1 < \epsilon_2 < \dots < \epsilon_{d_S}$$

- We suppose **energy differences** to be also non degenerate

$$\epsilon_i - \epsilon_j = \epsilon_m - \epsilon_n \quad \Leftrightarrow \quad \begin{cases} i = m \ \& \ j = n \\ i = j \ \& \ m = n \end{cases}$$

Bohr frequencies

$$\omega_{\ell(i,j)} = \epsilon_i - \epsilon_j \quad i, j = 1, \dots, d_S$$

under our assumptions

$$\text{ordered pair } (i, j) \ i \neq j \quad \Longleftrightarrow \quad -L \leq \ell \leq L$$

vHSL: truncation of the Born series

Nakajima-Zwanzig equation initial data at $t = t_\ell$

$$\partial_t \tilde{\rho}_t^{(S)} = -\text{Tr}_{\mathcal{H}^{(E)}} \left(\int_{t_\ell}^t ds \mathfrak{P} \left(\left[\tilde{\mathbf{H}}_t^{(\iota)}, G_{t,s} \left[\tilde{\mathbf{H}}_s^{(\iota)}, \tilde{\rho}_s^{(S)} \otimes \rho_{t_\ell}^{(E)} \right] \right] \right) \right)$$

Weak coupling: $\tilde{\mathbf{H}}_s^{(\iota)} \propto g$ & $g \ll 1$

$$G_{t,s} = 1_{\mathcal{H}^{(S)} \otimes \mathcal{H}^{(E)}} + O(g)$$

$$\Rightarrow \partial_t \tilde{\rho}_t^{(S)} = -\text{Tr}_{\mathcal{H}^{(E)}} \left(\int_0^t ds \mathfrak{P} \left(\left[\tilde{\mathbf{H}}_t^{(\iota)}, \left[\tilde{\mathbf{H}}_s^{(\iota)}, \tilde{\rho}_s^{(S)} \otimes \rho_{t_\ell}^{(E)} \right] \right] \right) \right) + O(g^3)$$

Self-adjoint and trace preserving equation for $\sigma_t \in \mathcal{M}_{d_S}(\mathbb{C})$

$$\partial_t \sigma_t = \int_{t_\ell}^t ds \left(\mathfrak{G}_{t,s,t_\ell}(\sigma_s) + (\mathfrak{G}_{t,s,t_\ell}(\sigma_s))^\dagger \right)$$

$$\mathfrak{G}_{t,s,t_\ell}(\sigma_s) = \text{Tr}_{\mathcal{H}^{(E)}} \left(\tilde{\mathbf{H}}_s^{(\iota)} \sigma_s \otimes \rho_{t_\ell}^{(E)} \tilde{\mathbf{H}}_t^{(\iota)} - \tilde{\mathbf{H}}_t^{(\iota)} \tilde{\mathbf{H}}_s^{(\iota)} \sigma_s \otimes \rho_{t_\ell}^{(E)} \right)$$

vHSL: Insertion of the explicit expression of the interaction

We decompose the $A^{(a)}$'s in outer products of $H^{(S)}$ eigenstates

$$\tilde{H}_t^{(\iota)} = g \sum_{a=1}^N \sum_{\ell=-L}^L e^{i \omega_{\ell} t} A_{\ell}^{(a)} \otimes e^{i H^{(E)} t} B^{(a)} e^{-i H^{(E)} t}$$

Consequence for the generator

$$\mathfrak{G}_{t,t_{\iota}}(\sigma_t) + (\mathfrak{G}_{t,t_{\iota}}(\sigma_t))^{\dagger} =$$

$$g^2 \operatorname{Re} \left(\sum_{\ell, \ell'=-L}^L \sum_{a, a'=1}^N \left(A_{\ell'}^{(a')} \sigma_t A_{\ell}^{(a) \dagger} - A_{\ell}^{(a) \dagger} A_{\ell'}^{(a')} \sigma_t \right) e^{-i (\omega_{\ell} - \omega_{\ell'}) t} \Gamma_{\ell'}^{(a, a')} \right)$$

Bath correlations: the limit **requires** $\dim(\mathcal{H}^{(E)}) = \infty$

$$\frac{\Gamma_{\ell'}^{(a, a')}}{2} = \lim_{t_{\iota} \downarrow -\infty} \int_0^{t-t_{\iota}} ds e^{-i \omega_{\ell} s} \operatorname{Tr} \left(e^{i H^{(E)} s} B^{(a)} e^{-i H^{(E)} s} \rho_{t_{\iota}}^{(E)} B^{(a')} \right)$$

vHLS: dependence on Bohr frequencies

After some algebra

$$\partial_t \sigma_t = -i [H_t^{(LS)}, \sigma_t] + g^2 \sum_{\ell, \ell'=-L}^L e^{-i(\omega_\ell - \omega_{\ell'})t} \sum_{a, a'=1}^N R_{\ell, \ell'}^{(a, a')} \mathfrak{L}_{\ell, \ell'}^{(a, a')}(\sigma_t)$$

$$H_t^{(LS)} = g^2 \sum_{\ell, \ell'=-L}^L e^{-i(\omega_\ell - \omega_{\ell'})t} \sum_{a, a'=1}^N S_{\ell, \ell'}^{(a, a')} A_\ell^{(a)\dagger} A_{\ell'}^{(a')}$$

$$\mathfrak{L}_{\ell, \ell'}^{(a, a')}(\sigma_t) = A_{\ell'}^{(a')} \sigma_t A_\ell^{(a)\dagger} - \frac{A_\ell^{(a)\dagger} A_{\ell'}^{(a')} \sigma_t + \sigma_t A_\ell^{(a)\dagger} A_{\ell'}^{(a')}}{2}$$

$$R_{\ell, \ell'}^{(a, a')} = \frac{\Gamma_\ell^{(a, a')} + \overline{\Gamma_{\ell'}^{(a', a)}}}{2}$$

$$S_{\ell, \ell'}^{(a, a')} = \frac{\Gamma_\ell^{(a, a')} - \overline{\Gamma_{\ell'}^{(a', a)}}}{2i}$$

Does this equation preserve positivity? Not in general ...

vHLS: secular (rotating wave) approximation

Integral equation version with time rescaling

$$\sigma_t - \sigma_{t_\iota} = \int_0^{g^2(t-t_\iota)} ds \left(\frac{1}{i} \left[H_{\frac{s+t_\iota}{g^2}}^{(LS)}, \sigma_{\frac{s+t_\iota}{g^2}} \right] + \sum_{\ell, \ell'=-L}^L e^{-i(\omega_\ell - \omega_{\ell'}) \frac{s+t_\iota}{g^2}} F_{\ell, \ell'} \left(\sigma_{\frac{s+t_\iota}{g^2}} \right) \right)$$

$$F_{\ell, \ell'}(\sigma) = \sum_{a, a'=1}^N R_{\ell, \ell'}^{(a, a')} \left(A_{\ell'}^{(a')} \sigma A_\ell^{(a) \dagger} - \frac{A_\ell^{(a) \dagger} A_{\ell'}^{(a')} \sigma + \sigma A_\ell^{(a) \dagger} A_{\ell'}^{(a')}}{2} \right)$$

Enters the Riemann-Lebesgue theorem

if we assume $\lim_{\substack{g \downarrow 0 \\ t_\iota \downarrow -\infty}} \sigma_t = \varsigma_\tau$ holding $\tau = g^2(t - t_\iota)$ finite

$$\varsigma_\tau - \sigma_\star = \int_0^\tau ds \left(\frac{1}{i} \left[H_\star^{(LS)}, \varsigma_s \right] + \sum_{\ell=-L}^L F_{\ell, \ell}(\varsigma_s) \right)$$

then

$$H_\star^{(LS)} = \sum_{\ell=-L}^L \sum_{a, a'=1}^N S_{\ell, \ell}^{(a, a')} A_\ell^{(a) \dagger} A_\ell^{(a')}$$

vHSL: the CP master equation in Dirac's picture

First canonical form: $R_{\ell,\ell}^{(a,a')} \equiv W_{\ell}^{(a,a')}$

$$\partial_{\tau} \varsigma_{\tau} = -i [H_{\star}^{(LS)}, \varsigma_{\tau}] + \sum_{\ell=-L}^L \sum_{a,a'=1}^N \mathbf{W}_{\ell}^{(a,a')} \left(A_{\ell}^{(a')} \varsigma_{\tau} A_{\ell}^{(a)\dagger} - \frac{A_{\ell}^{(a)\dagger} A_{\ell}^{(a')} \varsigma_{\tau} + \varsigma_{\tau} A_{\ell}^{(a)\dagger} A_{\ell}^{(a')}}{2} \right)$$

Q: For any ℓ do the $R_{\ell,\ell}^{(a,a')}$ specify a **positive** matrix?

by definition

$$W_{\ell}^{(a,a')} = \lim_{t_l \downarrow -\infty} \int_{t_l}^{|t_l|} ds e^{i\omega_{\ell}s} \text{Tr} \left(e^{i H^{(E)} s} B^{(a)} e^{-i H^{(E)} s} B^{(a')} \rho_{t_l}^{(E)} \right)$$

by direct calculation

$$\begin{aligned} & \sum_{a,a'=1}^N \bar{c}_a \text{Tr} \left(e^{i H^{(E)} s} B^{(a)} e^{-i H^{(E)} s} B^{(a')} \rho_{t_l}^{(E)} \right) c_{a'} \\ &= \text{Tr} \left(\left| \sum_{a=1}^N e^{-i H^{(E)} s} B^{(a)} c_a \right|^2 \rho_{t_l}^{(E)} \right) \geq 0 \quad \mathbf{A: YES!!!} \end{aligned}$$

vHSL: the CP master equation in Schrödinger's picture

$$U_t = \exp(-i H^{(S)} (t - t_\iota))$$

$$\partial_t \rho_t = -i [H^{(S)} + H_\star^{(LS)}, \rho_t]$$

$$+ \sum_{\ell=-L}^L \sum_{a,a'=1}^N W_\ell^{(a,a')} \left(A_\ell^{(a')} \rho_t A_\ell^{(a)\dagger} - \frac{A_\ell^{(a)\dagger} A_\ell^{(a')} \rho_t + \rho_t A_\ell^{(a)\dagger} A_\ell^{(a')}}{2} \right)$$

- To go back to the Schrödinger picture we are “confusing” t with τ .
- The **exact** Nakajima-Zwanzig projection **commutes** with a rotation to the interaction picture.
- The **approximate treatment** relies on Riemann-Lebesgue and the introduction of $\tau = g^2 (t - t_\iota)$: performing these approximations in the interaction picture may not be equivalent to performing them in the Schrödinger picture.

Properties of the vHSL (Davies) CP master equation

KMS \implies **steady state is thermal** $\rho_\infty = e^{-\beta H^{(S)}} / Z^{(S)}$

$$\partial_t \rho_t = -i [H^{(S)} + H_\star^{(LS)}, \rho_t] + \sum_{\ell=-L}^L \sum_{a,a'=1}^N W_\ell^{(a,a')} \left(A_\ell^{(a')} \rho_t A_\ell^{(a)\dagger} - \frac{A_\ell^{(a)\dagger} A_\ell^{(a')} \rho_t + \rho_t A_\ell^{(a)\dagger} A_\ell^{(a')}}{2} \right)$$

- $[H^{(S)}, A_\ell^{(a')}] = \omega_\ell A_\ell^{(a')}$ since they are outer products of $H^{(S)}$ eigenstates
- If the initial **environment state operator is thermal** then correlation functions satisfy the Kubo-Martin-Schwinger (KMS) relation:

$$h_\ell^{(a,a')}(t) = \text{Tr} \left(e^{i t H^{(E)}} B^{(a)} e^{-i t H^{(E)}} \frac{e^{-\beta H^{(E)}}}{Z} B^{(a')} \right) \\ \implies C_\ell^{(a,a')}(t) = C_\ell^{(a',a)}(-t - i\beta)$$

- If KMS hold true then $W_{-\ell}^{(a,a')} = e^{-\beta \omega_\ell} W_\ell^{(a',a)}$ (**detailed balance**)

Partial secular apprximation

Cattaneo et al., *New Journal of Physics* **21**, p. 113045, (2019). arXiv: 1906.08893

Trushechkin, *Physical Review A* **103**, p. 062226, (2021). arXiv: 2103.12042

Vaaranta and Cattaneo, *Eprint to appear*, (2025). arXiv: August.

For physical systems $0 < g \ll 1$ and $t_\ell > -\infty$

$$\varsigma_\tau - \sigma_\star \simeq \int_0^\tau ds \left(\frac{1}{i} \left[H_{\frac{s+t_\ell}{g^2}}^{(LS)}, \varsigma_s \right] + \sum_{\ell, \ell'=-L}^L e^{-i(\omega_\ell - \omega_{\ell'}) \frac{s+t_\ell}{g^2}} F_{\ell, \ell'}(\varsigma_s) \right)$$

$$F_{\ell, \ell'}(\sigma) = \sum_{a, a'=1}^N R_{\ell, \ell'}^{(a, a')} \frac{\left[A_\ell^{(a) \dagger}, \sigma A_{\ell'}^{(a')} \right] + \left[A_\ell^{(a) \dagger} \sigma, A_{\ell'}^{(a')} \right]}{2} \quad (\text{rewriting!})$$

- $\min_{\ell, a, a'} R_{\ell, \ell}^{(a, a')} = \tau_R^{-1}$
- $(\omega_\ell - \omega_{\ell'}) \frac{T_R}{g^2} \gg 1$ drop.
- $(\omega_\ell - \omega_{\ell'}) \frac{T_R}{g^2} \lesssim 1$ retain.

$$\partial_\tau \varsigma_\tau = \frac{1}{i} \left[H_\star^{(LS)}, \varsigma_s \right] + \sum_{\ell \in F_0} \sum_{a, a'=1}^N R_{\ell, \ell}^{(a, a')} \frac{\left[A_\ell^{(a) \dagger}, \varsigma_t A_{\ell'}^{(a')} \right] + \left[A_\ell^{(a) \dagger} \varsigma_t, A_{\ell'}^{(a')} \right]}{2}$$

A tale of several time-scales

Khalfin, *Doklady Akademii Nauk SSSR* **2**, p. 340, (1957).

Brown, *Quantum Field Theory*, Cambridge University Press, (1994). ch 6.3

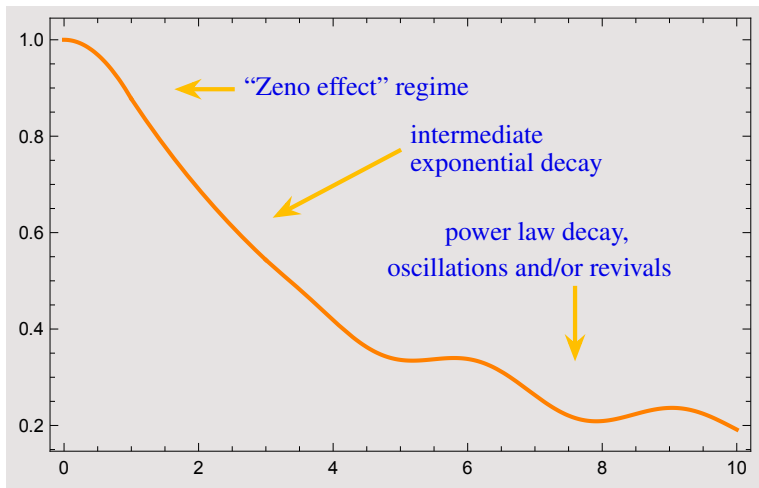


Figure: State survival probability under unitary evolution

Summary

- **Nakjima-Zwanzig** provides a non-perturbative framework to define open system dynamics (also in the classical case).
- **Time-convolutionless** perturbation theory permits systematic construction of master equation.
- **Positivity preservation** is often an issue.
- **The Davies master equation** obtained in the van Hove (or weak coupling) scaling limit yields is **completely positive**.
- **The Davies master equation** requires coupling to an infinite bath.
- Limitation of the van Hove scaling limit: $\tau = g^2 (t - t_\ell)$ means that time can be large only if g is very small.

Lecture III: Quantum Trajectories: Stochastic Processes in a System's Hilbert Space

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Summer School
on

New Directions in Quantum and Quantum Reservoir Computing,
Quantum Devices and Related Technologies

Aalto university - 18.–22.8.2025

Back to the postulates

I - Unitary evolution of the state vector: Schrödinger equation

$$\begin{cases} i \partial_t \psi_t = H \psi_t \\ \psi_0 = \psi_o \end{cases} \quad H^\dagger = H$$

II - The generalized measurement postulate

- Experiment with \mathcal{M} distinct possible outcomes.
- To the k -th outcome we associate an operator M_k on \mathcal{H} such that

$$\sum_{k=1}^{\mathcal{M}} M_k^\dagger M_k = 1_d \quad d = \dim \mathcal{H}$$

- If we observe the k -th outcome, the state collapses to a new value

$$\psi_t \rightarrow \psi_{t+dt} = \frac{M_k \psi_t}{\|M_k \psi_t\|}$$

"Quantum Jumps"

Two dynamics?

We *never* experiment with just one electron or atom or (small) molecule. In thought-experiments we sometimes assume that we do; this invariably entails ridiculous consequences.

Erwin Schrödinger, “Are there Quantum Jumps?”,
The British Journal for the Philosophy of Science, 1952.

As quoted in

Serge Haroche, and Jean-Michel Raimond,
“Exploring the Quantum: Atoms, Cavities, and Photons” Chap 1
Oxford Graduate Texts, 2006, X,616.

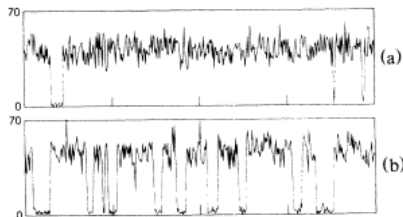
Observation of Quantum Jumps in a Single Atom

J. C. Bergquist, Randall G. Hulet, Wayne M. Itano, and D. J. Wineland

Time and Frequency Division, National Bureau of Standards, Boulder, Colorado 80303

(Received 23 June 1986)

We detect the radiatively driven electric quadrupole transition to the metastable $^2D_{5/2}$ state in a single, laser-cooled Hg II ion by monitoring the abrupt cessation of the fluorescence signal from the laser-excited $^2S_{1/2} \rightarrow ^2P_{1/2}$ first resonance line. When the ion “jumps” back from the metastable D state to the ground S state, the $S \rightarrow P$ resonance fluorescence signal immediately returns. The statistical properties of the quantum jumps are investigated; for example, photon antibunching in the emission from the D state is observed with 100% efficiency.



Wineland, *Reviews of Modern Physics* **85**, pp. 1103–1114, (2013).

2012 Nobel Prize in Physics

Serge Haroche and **David J. Wineland**, for “ground-breaking experimental methods that enable measuring and manipulation of *individual quantum systems*”

A lesson in life

Which goes to show that the best of us must sometimes eat our words.

*Albus P. W. B. Dumbledore
as quoted in*

J.K. Rowlings

*“Harry Potter and the Chamber of
Secrets” Chap 18*

Bloomsbury 1998.



Can we model a measurement record?

Srinivas and Davies, *Optica Acta: International Journal of Optics* **28**, (1981). .

Wiseman and Milburn, *Quantum Measurement and Control*, Cambridge University Press, (2009).

Key points

Measurement is a form of system-environment interaction.

Use the measurement postulate to infer the effective system dynamics.

Let ψ state vector of the system at time t .

Let in $(t, t + dt]$ the measurement admit only two **random** outcomes

1 “Null result” with probability (i.e close to one)

$$\| M_0 \psi_t \|^2 = 1 - E (d\nu_t | \psi_t, \bar{\psi}_t)$$

2 “Detection”

$$\| M_1 \psi_t \|^2 = E (d\nu_t | \psi_t, \bar{\psi}_t)$$

$E (d\nu_t | \psi_t, \bar{\psi}_t)$: expectation value of the increment of a counting process
conditional on the state of the system immediately before the jump

Counting process

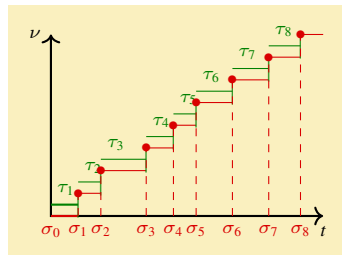
Klebaner, *Introduction to Stochastic Calculus with Applications*, Imperial College Press, (2005). ch 9

Breuer and Petruccione, *The Theory of Open Quantum Systems*, Oxford University Press, (2002). ch 1

Pure jump process $\nu_t = \sum_{i=1}^{\infty} 1_{[0,t]}(\sigma_i)$

Arrival process $\begin{cases} \sigma_0 = 0 \\ \sigma_n = \sum_{k=1}^n \tau_k \end{cases}$

Waiting times: τ_k positive random variables



Waiting time conditional on the state vector process

$$(d\nu_t)^2 = d\nu_t$$

$$\mathbb{E}(d\nu_t | \psi_t, \bar{\psi}_t) = \|\mathbf{R} \psi_t\|^2 dt$$

$$\Rightarrow \mathbf{M}_1 = \mathbf{R} \sqrt{dt}$$

	dt	$d\nu_t$
dt	0	0
$d\nu_t$	0	$d\nu_t$

Evolution of the state vector

State vector's **stochastic** update rule

$$\psi_{t+dt} = \psi_t + (1 - d\nu_t) \left(\frac{M_0 \psi_t}{\|M_0 \psi_t\|} - \psi_t \right) + d\nu_t \left(\frac{M_1 \psi_t}{\|M_1 \psi_t\|} - \psi_t \right)$$

Probability conservation & differential algebra

$$1 = \|M_0 \psi_t\|^2 + \|M_1 \psi_t\|^2 \quad \forall t \geq 0 \quad \& \quad \psi, \bar{\psi}$$

$$\Rightarrow M_0 = 1_d - \left(\textcolor{red}{i} H + \frac{R^\dagger R}{2} \right) dt + o(dt)$$

Main result: Itô stochastic differential equation

$$d\psi_t = -dt \left(\textcolor{red}{i} H + \frac{R^\dagger R - \|R \psi_t\|^2}{2} \right) \psi_t \\ + d\nu_t \left(\frac{R \psi_t}{\|R \psi_t\|} - \psi_t \right)$$

	Remember!	
	dt	dν _t
dt	0	0
dν _t	0	dν _t

Recovery of the master equation

Itô lemma for counting processes

$$d(\psi_t \psi_t^\dagger) = (d\psi_t) \psi_t^\dagger + \psi_t d\psi_t^\dagger + (d\psi_t) d\psi_t^\dagger$$

	Remember!	
	dt	$d\nu_t$
dt	0	0
$d\nu_t$	0	$d\nu_t$

Telescopic property of conditional expectation

$$\mathbb{E} \left(F(\psi_t, \bar{\psi}_t) d\nu_t \right) = \mathbb{E} \left(F(\psi_t, \bar{\psi}_t) \mathbb{E} \left(d\nu_t | \psi_t, \bar{\psi}_t \right) \right) = \mathbb{E} \left(F(\psi_t, \bar{\psi}_t) \|R \psi_t\|^2 \right) dt$$

$\rho_t = \mathbb{E}(\psi_t \psi_t^\dagger)$ satisfies a completely positive master equation

$$\partial_t \rho_t = -i [H, \rho_t] + R \rho_t R^\dagger - \frac{R^\dagger R \rho_t + \rho_t R^\dagger R}{2}$$

Proof: compute $d \mathbb{E}(\psi_t \psi_t^\dagger) = \mathbb{E} \left(d(\psi_t \psi_t^\dagger) \right)$

Stochastic Schrödinger equation (SSE) in canonical form

Barchielli and Belavkin, *Journal of Physics A: Mathematical and General* **24**, (1991).

Dalibard, Castin, and Mølmer, *Physical Review Letters* **68**, (1992). .

Donvil and Muratore-Ginanneschi, *Open Systems & Information Dynamics* **30**, (2023). arXiv: 2309.13408.

$\mathbf{r}_t^{(\ell)} \geq 0$: unraveling in quantum trajectories of the canonical form of the completely positive master equation

$$\rho_t = \mathbb{E} \psi_t \psi_t^\dagger \quad \text{unraveling of } \rho_t$$

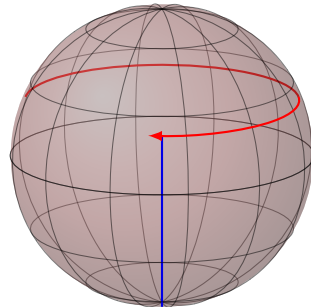
$$d\psi_t = dt K_t \psi_t + \sum_{\ell=1}^{d^2-1} d\nu_t^{(\ell)} \left(\frac{L_t^{(\ell)} \psi_t}{\|L_t^{(\ell)} \psi_t\|} - \psi_t \right)$$

$$K_t = -\frac{1}{2} H_t - \sum_{\ell=1}^{d^2-1} \mathbf{r}_t^{(\ell)} \frac{L_t^{(\ell) \dagger} L_t^{(\ell)} - \|L_t^{(\ell)} \psi_t\|^2 1_d}{2}$$

$$d\nu_t^{(\ell)} d\nu_t^{(\tilde{k})} = \delta_{\ell, \tilde{k}} d\nu_t^{(\ell)}$$

$$\ell, \tilde{k} = 1, \dots, d^2 - 1$$

$$\mathbb{E} (d\nu_t^{(\ell)} | \psi_t, \bar{\psi}_t) = \mathbf{r}_t^{(\ell)} \|L_t^{(\ell)} \psi_t\|^2 dt$$



Bloch hyper-sphere

Reconciling non-linearity with probability conservation

Barchielli and Belavkin, *Journal of Physics A: Mathematical and General* **24**, (1991).

Wiseman, *Quantum and Semiclassical Optics: Journal of the European Optical Society Part B* **8**, (1996).

Non linear evolution

$\|\psi_t\|^2 = 1$ along all stochastic paths on the Bloch hyper-sphere

Mapping to linear

- 1 Assume: $\psi_t = \frac{\varphi_t}{\|\varphi_t\|}$
- 2 Require: φ_t evolves linearly.
- 3 Plug into the SSE and do your math.
- 4 (Optional) redefine the counting process to be Poisson (Girsanov formula): $\varphi_t \mapsto \chi_t$ & $\nu_t^{(\ell)} \mapsto \pi_t^{(\ell)}$

$$d\chi_t = -K_t \chi_t dt + \sum_{\ell=1}^{\mathcal{L}} d\pi_t^{(\ell)} (L_t^{(\ell)} - 1_d) \chi_t$$

$$K_t = i H_t + \sum_{\ell=1}^{\mathcal{L}} \frac{r_t^{(\ell)}}{2} L_t^{(\ell) \dagger} L_t^{(\ell)}$$

- $\rho_t = \tilde{E} \chi_t \chi_t^\dagger$ (expectation w.r.t. $\pi_t^{(\ell)}$'s)

	dt	dν _t
dt	0	0
dν _t	0	dν _t

$$E(d\pi_t^{(\ell)}) = r_t^{(\ell)} dt$$

	dt	dπ _t
dt	0	0
dπ _t	0	dπ _t

Why unraveling the state operator?

Three reasons

Wiseman, *Quantum and Semiclassical Optics: Journal of the European Optical Society Part B* **8**, (1996).

- **Indirect** (continuous time, non-demolition) **measurement**: unraveling relates the statistics of individual random detection events to the state operator.

Example applications: **quantum state estimation** (Murch et al., *Nature* **502**, (2013). arXiv: 1305.7270. DianTan et al., *Physical Review Letters* **114**, (2015). arXiv: 1409.0510.), **feedback control** (Wiseman and Doherty, *Physical Review Letters* **94**, (2005). arXiv: quant-ph/0408099.) etc.

- **Numerical integration in high dimensional Hilbert spaces:**

N -state system	Real numbers to store per step	Expected computing time scaling
Direct integration of the master equation	$O(N^2)$	$O(N^4)$
Integration via unraveling	$O(2N)$	$O(\mathcal{N} \times N^2)$ $\mathcal{N} = \text{realizations} $

- **Foundational reason**: element of a still missing theory of quantum state reduction? Bassi and Ghirardi, *Physics Reports* **379**, (2003). arXiv: quant-ph/0302164.

The QuTiP algorithm in a Nutshell <https://qutip.org/>

Johansson, Nation, and Nori, *Computer Physics Communications* **184**, (2013). arXiv: 1110.0573.

Lambert et al., *Eprint*, April, (2024). arXiv: 2412.04705

- 1 Sample a random variable $\xi_1 : \Omega : \mapsto [0, 1]$: **jump time** (Step 3).
- 2 Sample a random variable $\xi_2 : \Omega : \mapsto [0, 1]$: **jump type** (Step 4).
- 3 Integrate $\dot{\psi}_t = -\mathbf{K}_t \psi_t$ from initial datum ψ_o at $t = 0$, using:

$$\mathbf{K}_t = i \mathbf{H}_t + \sum_{\ell=1}^{d^2-1} \frac{r_t^{(\ell)} \mathbf{L}^{(\ell) \dagger} \mathbf{L}_t^{(\ell)}}{2}$$

until the **jump time** $\tau = \min \{t \geq t_o \mid \|\psi_t\|^2 \leq \xi_1\}$

- 4 Collapse to state

$$\tilde{\psi}_{\tau}^{(n)} = \frac{\mathbf{L}_{\tau}^{(n)} \psi_{\tau}}{\|\mathbf{L}_{\tau}^{(n)} \psi_{\tau}\|} \quad (*)$$

$$n = \min \left\{ 1 \leq n \leq d^2 - 1 \mid \sum_{\ell=1}^n \|\mathbf{L}_{\tau}^{(\ell)} \psi_{\tau}\|^2 \geq \rho_2 \right\}$$

- 5 Repeat with new initial condition (*) at time $t = \tau$.

Quantum State diffusion

Percival, *Quantum State Diffusion*, Cambridge University Press, (2003).

Barchielli and Gregoratti, *Quantum Trajectories and Measurements in Continuous Time*, Springer, (2009).

Aggregate effect of jumps: $\psi_t, \bar{\psi}_t$ satisfy Itô SDEs

$$d\psi_t = -K_t \psi_t dt + \sum_{\ell=1}^{\mathcal{L}} dw_t^{(\ell)} \left(L_t^{(\ell)} - \text{Re} \left\langle \psi_t^\dagger, L_t^{(\ell)} \psi_t \right\rangle 1_d \right) \psi_t$$

$$K_t = i H_t + \sum_{\ell=1}^{\mathcal{L}} \frac{L_t^{(\ell) \dagger} L_t^{(\ell)} - 2 \text{Re} \left\langle \psi_t^\dagger, L_t^{(\ell)} \psi_t \right\rangle L_t^{(\ell)} + (\text{Re} \left\langle \psi_t, L_t^{(\ell)} \psi_t \right\rangle)^2}{2} 1_d$$

$$\psi_0 = \psi_o$$

		dt	$d\omega_t^{(a)}$	$d\bar{\omega}_t^{(a)}$	$d\omega_t^{(b)}$	$d\bar{\omega}_t^{(b)}$
• Gaussian processes	dt	0	0	0	0	0
• $E d\omega_t^{(\ell)} = 0$	$d\omega_t^{(a)}$	0	0	dt	0	0
• $E d\omega_t^{(\ell)} d\bar{\omega}_t^{(k)} = \delta_{\ell,k} dt$	$d\bar{\omega}_t^{(a)}$	0	dt	0	0	0
• $E d\omega_t^{(\ell)} d\omega_t^{(k)} = 0$	$d\omega_t^{(b)}$	0	0	0	0	dt
	$d\bar{\omega}_t^{(b)}$	0	0	0	dt	0

Quantum Filtering

Belavkin, *Radiotekhnika i Elektronika* **25**, (1980).

Gisin, *Physical Review Letters* **52**, (1984).

Jacobs, *Quantum Measurement Theory and its Applications*, Cambridge University Press, (2014).

Stochastic evolution of the state operator (canonical form)

$$\begin{aligned} d\varrho_t = & \left(-i [H_t, \varrho_t] + \sum_{\ell=1}^{\mathcal{L}} \left(L_t^{(\ell)} \varrho_t L_t^{(\ell)\dagger} - \frac{L_t^{(\ell)\dagger} L_t^{(\ell)} \varrho_t + \varrho_t L_t^{(\ell)\dagger} L_t^{(\ell)}}{2} \right) \right) dt \\ & + \sum_{\ell=1}^{\mathcal{L}} dw_t^{(\ell)} \left(L_t^{(\ell)} - \text{Re Tr} (L_t^{(\ell)} \varrho_t) 1_d \right) \varrho_t \\ & + \sum_{\ell=1}^{\mathcal{L}} d\bar{w}_t^{(\ell)} \varrho_t \left(L_t^{(\ell)\dagger} - \text{Re Tr} (L_t^{(\ell)\dagger} \varrho_t) 1_d \right) \\ \rho_0 = & \rho_o \end{aligned}$$

Quantum “counterpart” of the classical Kushner-Stratonovich equation

Canonical Nakajima-Zwanzig master equation

Master equation in canonical form

$$\partial_t \rho_t = -i [H_t, \rho_t] + \sum_{\ell=1}^{d^2-1} \frac{c_t^{(\ell)}}{2} ([L_t^{(\ell)}, \rho_t L_t^{(\ell)\dagger}] + [L_t^{(\ell)} \rho_t, L_t^{(\ell)\dagger}])$$

- $\text{Tr}(L_t^{(\ell)\dagger} L_t^{(k)}) = \delta_{\ell,k}$ and $\text{Tr}(L_t^{(k)}) = 0$
- The couplings of the Lindblad operators are bounded $|c_t^{(\ell)}| < \infty$
- The couplings of the Lindblad operators are **NOT** sign definite $c_t^{(\ell)} \not\leq 0$
- **Generates a completely bounded semi-group.** Canonical Wittstock-Paulsen form trace and self-adjoint preserving:

$$\rho_t = \sum_{a=1}^{\mathcal{N}^{(+)}} V_{t,t_\ell}^{(a)} \rho_{t_\ell} V_{t,t_\ell}^{(a)\dagger} - \sum_{a=1}^{\mathcal{N}^{(-)}} W_{t,t_\ell}^{(a)} \rho_{t_\ell} W_{t,t_\ell}^{(a)\dagger}$$

Q: Is there a stochastic representation? Some approaches

- Breuer, *Physical Review A* **70**, (2004). arXiv: quant-ph/0403117. (embedding in CP master equation)
- Piilo et al., *Physical Review Letters* **100**, (2008). arXiv: 0706.4438. (algorithm)
- Settimo et al., *Physical Review A* **109**, (2024). arXiv: 2402.12445. (rate equations)

Canonical unraveling by the influence martingale

Donvil and Muratore-Ginanneschi, *Nature Communications* **13**, (2022). arXiv: 2102.10355.

Donvil and Muratore-Ginanneschi, *New Journal of Physics* , (2023). arXiv: 2209.08958.

Donvil and Muratore-Ginanneschi, *Open Systems & Information Dynamics* **30**, (2023).

$$\rho_t = \mathbb{E} \left(\mu_t \psi_t \psi_t^\dagger \right)$$

$$\mu_t^{(\pm)} = \max(0, \pm \mu_t) \quad \Rightarrow \quad \rho_t = \mathbb{E} \left(\mu_t^{(+)} \psi_t \psi_t^\dagger - \mu_t^{(-)} \psi_t \psi_t^\dagger \right)$$

The triple $(\mu_t, \psi_t, \psi_t^\dagger)$ is a Markov process.

ψ_t obeys the standard stochastic Schrödinger equation with $\|\psi_t\|^2 = 1$ driven by counting processes:

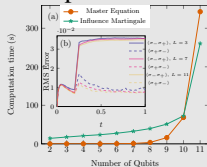
$$\varrho_t = \mathbb{E} \left(\psi_t \psi_t^\dagger \right)$$

solves a **dual** Lindblad equation.

μ_t **mean preserving** stochastic process (=martingale). A path of μ_t depends only on **one** path of ψ_t, ψ_t^\dagger

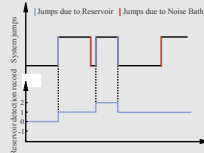
Some applications

Simulation of spin chains



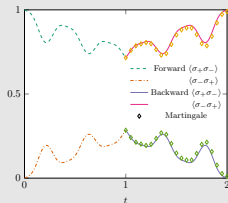
Donvil and Muratore-Ginanneschi, *Nature Communications* **13**, (2022).

Quantum Error Mitigation: jump cancellation by post-processing



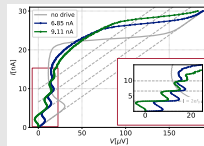
Donvil et al., *Physical Review A* **111**, (2023). arXiv: 2305.19874.

Inversion of completely positive maps



Donvil and Muratore-Ginanneschi, *New Journal of Physics*, (2023).

Metrology: solution of stylized models of inverse Shapiro steps



Resch et al., *Eprint*, (2025). arXiv: 2508.04574.

Numerical implementation in QuTip 5

Influence martingale toolkit included in package 'nm_solve'

DOCs & tutorials https://github.com/qutip/qutip-tutorials/blob/main/tutorials-v5/time-evolution/013_nonmarkovian_monte_carlo.md

Summary

- Open classical systems: stochastic processes and viscous hydrodynamics:
 - “Eulerian picture”: evolution of the probability distribution.
 - “Lagrangian picture”: stochastic evolution of a point particle or fluid element: stochastic differential equations (SDE).

Equivalent pictures but **depending on the problem** one may be more suited than the other to offer insights. **MonteCarlo methods based on SDEs are advantageous to tackle the curse of dimensionality.**

- Open quantum systems:
 - master equation: deterministic evolution of the state **operator**.
 - quantum trajectories: stochastic evolution of the state **vector**.

The difference with respect to the classical case resides in the relation

$$\rho_t = \mathbb{E} (\mu_t \psi_t \psi_t) \quad \begin{array}{l} \psi_t \text{ stochastic process on the Hilbert space} \\ \mu_t \text{ martingale process eventually } = 1 \end{array}$$

otherwise the rationale for adopting one or the other picture of the dynamics is the same as in the classical case. Unless...

THANKS!