Quantum master equations are unraveled by Markov processes

Paolo Muratore-Ginanneschi (U.H.)

based on joint work with

Brecht Donvil (Ulm University)

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Department of Mathematics and Statistics
University of Helsinki

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Evolution of an open quantum system state operator

$$\rho_t = \Phi_{t\,t_\circ}(\rho_{t_\circ}) \qquad \text{from microscopic unitary dynamics}$$

- Completely positive dynamical map: existence of a time $t_\circ$ when the state operator is in tensor product form:

$$\Phi_{t\,t_\circ}(\rho_{t_\circ}) = \mathrm{Tr}_{\mathcal{H}_E}\left(\mathrm{U}_{t\,t_\circ}\,\rho_{t_\circ} \otimes \sigma_{t_\circ}\,\mathrm{U}^\dagger_{t\,t_\circ}\right)$$

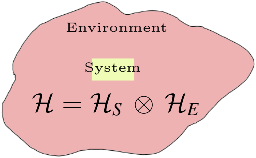
$\sigma_{t_\circ}$ environment

$\rho_{t_\circ}$ system

- Complete positive map $\Leftrightarrow$ Choi-Stinespring repr.:

$$\Phi_{t\,t_\circ}(\rho_{t_\circ}) = \sum_i \mathrm{V}_{i,t\,t_\circ}\,\rho_{t_\circ}\,\mathrm{V}^\dagger_{i,t\,t_\circ}$$

$$\sum_i \mathrm{V}^\dagger_{i,t\,t_\circ}\,\mathrm{V}_{i,t\,t_\circ} = 1_{\mathcal{H}} \qquad \text{(trace preserving)}$$



- Obs: the inverse (if any) of a completely positive map is not necessarily completely positive!

Completely positive $\neq$ completely positive divisible

- If a dynamical map $\boldsymbol{\Phi}_{t\,t_\circ}$ is invertible at any time, then it is also divisible

Breuer et al., *Reviews of Modern Physics*, (2016)

$$\boldsymbol{\Phi}_{t\,s} = \boldsymbol{\Phi}_{t\,t_\circ}\boldsymbol{\Phi}_{s\,t_\circ}^{-1}$$

- If $\boldsymbol{\Phi}_{t\,s}$ is divisible then we can define an infinitesimal generator:

$$\boldsymbol{\Phi}_{t+\varepsilon\,s} - \boldsymbol{\Phi}_{t\,s} = (\boldsymbol{\Phi}_{t+\varepsilon\,t} - 1)\,\boldsymbol{\Phi}_{t\,s} = \mathrm{G}_t(\boldsymbol{\Phi}_{t\,s})\,\varepsilon + o(\varepsilon)$$

- Universal form of a linear trace preserving generator:

$$\mathrm{G}_t(\boldsymbol{\rho}_t) = -\imath\,[\mathrm{H}\,,\boldsymbol{\rho}_t] + \sum_{\ell=1}^{\mathscr{L}} \Gamma_{\ell,t}\left(\mathrm{L}_\ell\;\boldsymbol{\rho}_t\;\mathrm{L}_\ell^\dagger - \frac{\mathrm{L}_\ell^\dagger\,\mathrm{L}_\ell\;\boldsymbol{\rho}_t + \boldsymbol{\rho}_t\,\mathrm{L}_\ell^\dagger\,\mathrm{L}_\ell}{2}\right).$$

- The fundamental solution is completely positive iff

$$\Gamma_{\ell,t} \geq 0 \qquad \ell = 1,\dots,\mathscr{L} \qquad \& \qquad \forall\, t$$

Lindblad-Gorini-Kossakowski-Sudarshan master equation Lindblad, *Communications in Mathematical Physics*, (1976), Gorini et al., *Journal of Mathematical Physics*, (1976)

- $\Gamma_{\ell,t} \geq 0$ generate a completely positive dynamics.
- Rigorously derived in the weak coupling scaling limit Davies, *Quantum Theory of Open Systems*, (1976)

Why weak coupling provides a "sufficient condition" ?

- Exponential decay of survival probabilities in Q.M. only possible as **intermediate** asymptotics Khalfin, *Doklady Akademii Nauk SSSR*, (1957).
- Weak coupling scaling limit rivets on such intermediate asymptotics.
- $0 \leq \Gamma_{\ell,t} \sim$ probability per unit of time.

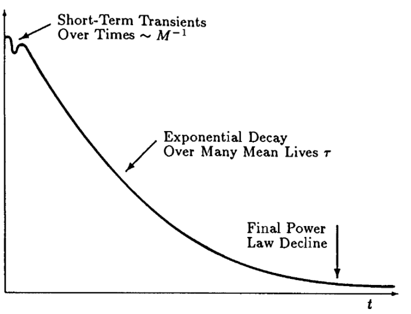


figure from Brown, *Quantum field theory*, (1994): continuous specrum etc.

Unraveling in the system's Hilbert space

$\Gamma_{\ell,t} \geq 0$: representation of the state operator as an average over state vector random paths in the system's Hilbert space Barchielli and Belavkin, *J. Phys. A: Math. Gen. 24 (1991) 1495–1514*, (2005), Dalibard, Castin, and Mølmer, *Physical Review Letters*, (1992)

$$\boldsymbol{\rho}_t = \mathrm{E}\, \boldsymbol{\psi}_t \boldsymbol{\psi}_t^{\dagger} \qquad \text{unraveling of } \boldsymbol{\rho}_t$$

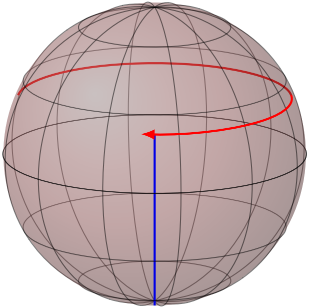
$$\mathrm{d}\,\boldsymbol{\psi}_t = \mathrm{d}t\, \boldsymbol{f}_t + \sum_{\ell=1}^{\mathscr{L}} \mathrm{d}\nu_{\ell,t} \left(\frac{\mathrm{L}_\ell\, \boldsymbol{\psi}_t}{\|\mathrm{L}_\ell\, \boldsymbol{\psi}_t\|} - \boldsymbol{\psi}_t \right)$$

$$\boldsymbol{f}_t = -\imath\, \mathrm{H}\, \boldsymbol{\psi}_t - \sum_{\ell=1}^{\mathscr{L}} \Gamma_{\ell,t} \frac{\mathrm{L}_\ell^{\dagger}\, \mathrm{L}_\ell\, \boldsymbol{\psi}_t - \|\mathrm{L}_\ell\, \boldsymbol{\psi}_t\|^2\, \boldsymbol{\psi}_t}{2}$$

$$\mathrm{d}\nu_{\ell,t}\mathrm{d}\nu_{\hbar,t} = \delta_{\ell,\hbar}\mathrm{d}\nu_{\ell,t}$$

$$\mathrm{E}\left(\mathrm{d}\nu_{\ell,t} \middle| \boldsymbol{\psi}_t, \bar{\boldsymbol{\psi}}_t\right) = \Gamma_{\ell,t}\, \|\mathrm{L}_\ell\, \boldsymbol{\psi}_t\|^2\, \mathrm{d}t$$

$$\ell, \hbar = 1, \ldots, \mathscr{L}$$



The role of complete positivity in unraveling

$$\mathrm{d}\boldsymbol{\rho}_t = \mathrm{E}\left((\mathrm{d}\boldsymbol{\psi}_t)\boldsymbol{\psi}_t^\dagger + \boldsymbol{\psi}_t \mathrm{d}\boldsymbol{\psi}_t^\dagger + (\mathrm{d}\boldsymbol{\psi}_t)(\mathrm{d}\boldsymbol{\psi}_t^\dagger)\right)$$

	$\mathrm{d}t$	$\mathrm{d}\nu_{\Bbbk,t}$
$\mathrm{d}t$	0	0
$\mathrm{d}\nu_{\ell,t}$	0	$\delta_{\ell\Bbbk}\mathrm{d}\nu_{\ell t}$

- Weighing factors $\Gamma_{\ell,t}$ identified as jump rates.
- Upon taking the expectation value "E"

$$\mathrm{E}(\mathrm{d}\boldsymbol{\psi}_t)(\mathrm{d}\boldsymbol{\psi}_t^\dagger) = \sum_{\ell=1}^{\mathscr{L}} \mathrm{E}\left(\mathrm{E}(\mathrm{d}\nu_{\ell,t}|\boldsymbol{\psi}_t,\bar{\boldsymbol{\psi}}_t)\left(\frac{\mathrm{L}_\ell\,\boldsymbol{\psi}_t}{\|\mathrm{L}_\ell\,\boldsymbol{\psi}_t\|} - \boldsymbol{\psi}_t\right)\left(\frac{\mathrm{L}_\ell\,\boldsymbol{\psi}_t}{\|\mathrm{L}_\ell\,\boldsymbol{\psi}_t\|} - \boldsymbol{\psi}_t\right)^\dagger\right)$$

- Prefactor of $\mathrm{L}_\ell\,\boldsymbol{\rho}_t\,\mathrm{L}_\ell^\dagger$ terms in the master equation positive by costruction.

Why unraveling the state operator?

Three reasons

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

- Indirect (continuous time) measurement: unraveling relates the statistics of individual random detection events to the state operator. Application example: quantum state parameter prediction and retrodiction.

- 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	$O(2N)$	$O(\mathcal{N} \times N^2)$ $\mathcal{N} = \#$ (realizations)

- Foundational reason: element of a still missing theory of quantum state reduction? Bassi and Ghirardi, *Physics Reports*, (2003)

Master equations from microscopic dynamics

The $\Gamma_{\ell,t}$'s may take **negative** values.

- Exact master equations from certain integrable models (e.g. spontaneous emission near the edge of a photonic band gap John and Quang, *Physical Review A*, (1994)).
- Exact master equations from Gaussian models (e.g. central boson/fermion model Tu and Zhang, *Physical Review B*, (2008)).
- Master equations generated by time convolutionless perturbation theory (Hashitsumae, Shibata, and Shingū, *Journal of Statistical Physics*, (1977)).

Survival probability at strong coupling

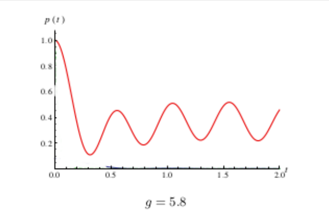


figure from Wolkanowski, "Resonances and poles in the second Riemann sheet", (2013)

Is it possible to unravel non-completely positive dynamics?

Stochastic unravelling in the doubled Hilbert space Breuer, Kappler, and Petruccione, *Physical Review A*, (1999)

$$\boldsymbol{\Psi}_t = \begin{bmatrix} \psi_t \\ \varphi_t \end{bmatrix} \qquad \& \qquad \boldsymbol{\rho}_t = \mathrm{E}\, \psi_t \varphi_t^\dagger$$

- $\boldsymbol{\Psi}_t$ obeys an ordinary stochastic differential equation with Poisson noise
- Proliferation of degrees of freedom

"Non Markovian" Monte Carlo wave function Piilo et al., *Physical Review Letters*, (2008)

- Evolution in the Hilbert space of the system
- state vector evolution NOT governed by ordinary stocastic differential equations
- algorithm keeps memory of jumps to produce "reversed " jumps.

Completely bounded divisible dynamics

Master equation

$$\partial_t \boldsymbol{\rho}_t = -\imath\, [\mathrm{H}_t\,, \boldsymbol{\rho}_t] + \sum_{\ell=1}^{\mathscr{L}} \frac{w_{\ell,t}}{2} \left(\left[\mathrm{L}_\ell\,, \boldsymbol{\rho}_t\, \mathrm{L}_\ell^\dagger \right] + \left[\mathrm{L}_\ell\, \boldsymbol{\rho}_t\,, \mathrm{L}_\ell^\dagger \right] \right).$$

- The weights of the Lindblad operators are bounded $|w_{\ell,t}| < \infty$
- The weights of the Lindblad operators are **NOT** sign definite $w_{\ell,t} \lesseqgtr 0$
- **The fundamental solution is a completely bounded map (CBM)**

CBM canonical form: Wittstock-Paulsen decomposition Wittstock, *Journal of Functional Analysis*, (1981) Paulsen, *Proceedings of the American Mathematical Society*, (1982) Paulsen, *Completely Bounded Maps and Operator Algebras*, (2003)

$$\boldsymbol{\rho}_t = \sum_{a=1}^{\mathscr{N}^{(+)}} \mathrm{V}_{a,t\,t_\circ}^{(+)}\, \boldsymbol{\rho}_{t_\circ}\, \mathrm{V}_{a,t\,t_\circ}^{(+)\dagger} - \sum_{a=1}^{\mathscr{N}^{(-)}} \mathrm{V}_{a,t\,t_\circ}^{(-)}\, \boldsymbol{\rho}_{t_\circ}\, \mathrm{V}_{a,t\,t_\circ}^{(-)\dagger}$$

Physics interpretation: compatibility domain problem Pechukas, *Physical Review Letters*, (1994), Shaji and Sudarshan, *Physics Letters A*, (2005), Hartmann and Strunz, *Physical Review A*, (2020)

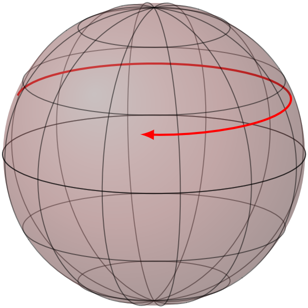
Unraveling by the influence martingale arXiv:2102.10355

The unraveling Ansatz: $\boldsymbol{\rho}_t = \mathrm{E}\, \mu_t \boldsymbol{\psi}_t \boldsymbol{\psi}_t^{\dagger}$

$$\mathrm{d}\, \boldsymbol{\psi}_t = \mathrm{d}t \boldsymbol{f}_t + \sum_{\ell=1}^{\mathscr{L}} \mathrm{d}\nu_{\ell,t} \left(\frac{\mathrm{L}_\ell\, \boldsymbol{\psi}_t}{\|\mathrm{L}_\ell\, \boldsymbol{\psi}_t\|} - \boldsymbol{\psi}_t \right)$$

$$\mathrm{d}\mu_t = \mu_t \sum_{\ell=1}^{\mathscr{L}} \left(\frac{w_{\ell,t}}{r_{\ell,t}} - 1 \right) \mathrm{d}\iota_{\ell,t}$$

$$\boldsymbol{f}_t = -\imath\, \mathrm{H}\, \boldsymbol{\psi}_t - \sum_{\ell=1}^{\mathscr{L}} w_{\ell,t} \frac{\mathrm{L}_\ell^{\dagger}\, \mathrm{L}_\ell\, \boldsymbol{\psi}_t - \|\mathrm{L}_\ell\, \boldsymbol{\psi}_t\|^2\, \boldsymbol{\psi}_t}{2}$$



$$\mathrm{E}\left(\mathrm{d}\nu_{\ell,t} \middle| \boldsymbol{\psi}_t, \bar{\boldsymbol{\psi}}_t \right) = r_{\ell,t}\, \|\mathrm{L}_\ell\, \boldsymbol{\psi}_t\|^2\, \mathrm{d}t$$

$$\mathrm{d}\iota_{\ell,t} = \mathrm{d}\nu_{\ell,t} - \mathrm{E}\left(\mathrm{d}\nu_{\ell,t} \middle| \boldsymbol{\psi}_t, \bar{\boldsymbol{\psi}}_t \right)$$

$$\mathrm{d}\nu_{\ell,t}\mathrm{d}\nu_{k,t} = \delta_{\ell,k}\mathrm{d}\nu_{\ell,t}$$

for $\ell, k = 1, \ldots, \mathscr{L}$

Proof

Just apply textbook rules of stochastic calculus for Poisson white noise:

Martingale property

$$\mathrm{d}\boldsymbol{\rho}_t = \mathrm{d}\left(\mathrm{E}\,\mu_t \psi_t \psi_t^\dagger\right) = \mathrm{E}\left(\cancel{(\mathrm{d}\mu_t)\psi_t\psi_t^\dagger} + \mu_t \mathrm{d}(\psi_t\psi_t^\dagger) + (\mathrm{d}\mu_t)\mathrm{d}(\psi_t\psi_t^\dagger)\right)$$

Recovery of the master equation

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E}(\mu_t\psi_t\psi_t^\dagger) = -\imath\,[\mathrm{H}\,,\boldsymbol{\rho}_t] \\
&-\sum_{\ell=1}^{\mathscr{L}} w_{\ell,t}\frac{\mathrm{L}_\ell^\dagger\,\mathrm{L}_\ell\,\boldsymbol{\rho}_t + \boldsymbol{\rho}_t\,\mathrm{L}_\ell^\dagger\,\mathrm{L}_\ell}{2} + \sum_{\ell=1}^{\mathscr{L}}\left(1+\left(\frac{w_{\ell,t}}{r_{\ell,t}}-1\right)\right) r_{\ell,t}\,\mathrm{L}_\ell\,\boldsymbol{\rho}_t\,\mathrm{L}_\ell^\dagger \\
&-\sum_{\ell=1}^{\mathscr{L}}\left(\left(1+\left(\frac{w_{\ell,t}}{r_{\ell,t}}-1\right)\right) r_{\ell,t} - w_{\ell,t}\right)\mathrm{E}(\|\mathrm{L}_\ell\,\psi_t\|^2\,\mu_t\psi_t\psi_t^\dagger)
\end{aligned}$$

Why the influence martingale?

Stochastic Wittstock–Paulsen decomposition

The unraveling enjoys the Markov property

$$\mu_t^{(\pm)} = \max(0, \pm\mu_t)$$

hence at any t

$$\boldsymbol{\rho}_t = \mathrm{E}\left(\mu_t^{(+)}\psi_t\boldsymbol{\psi}_t^{\dagger} - \mu_t^{(-)}\psi_t\boldsymbol{\psi}_t^{\dagger}\right)$$

- The influence is needed because a completely bounded state vector must be computed as the statistical average of terms reproducing the Wittstock-Paulsen decomposition
- In the completely positive case reduces to a (trivial) change of measure (Girsanov formula).

Evolution of the state vector

State vector evolution preserves the Bloch hyper-sphere

$$\mathrm{d}\left(\|\psi_t\|^2\right) = \sum_{\ell=1}^{\mathscr{L}} \left(\mathrm{d}\nu_{\ell,t} - w_{\ell,t}\,\|\mathrm{L}_\ell\,\psi_t\|^2\,\mathrm{d}t\right)\left(1 - \|\psi_t\|^2\right)$$

$$\mathrm{d}\mu_t = \mu_t \sum_{\ell=1}^{\mathscr{L}} \left(\frac{w_{\ell,t}}{r_{\ell,t}} - 1\right)\left(\mathrm{d}\nu_{\ell,t} - \mathrm{E}\left(\mathrm{d}\nu_{\ell,t}\middle|\psi_t, \bar{\psi}_t\right)\right)$$

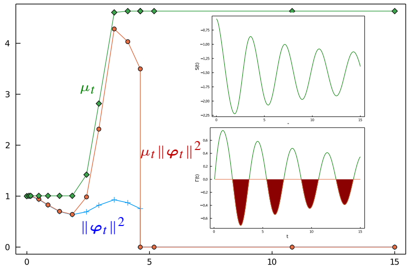
weights and rates

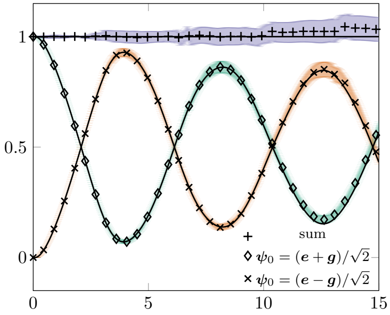
- Weights $\{w_{\ell,t}\}_{\ell=1}^{\mathscr{L}}$ predicted by theoretical calculation from the microscopic model
- Rates $\{r_{\ell,t}\}_{\ell=1}^{\mathscr{L}}$ inferred from measurement: contextual to unraveling.
- It is always possible to find a choice of $\{r_{\ell,t}\}_{\ell=1}^{\mathscr{L}}$ such that $\mathrm{E}\,\psi_t\psi_t^\dagger$ satisfies a LGKS equation.

Photonic band gap John and Quang, *Physical Review A*, (1994)

Exact master equation, violates Kossakowski conditions

$$\dot{\boldsymbol{\rho}}_t = \frac{S_t}{2\,\imath}\left[\sigma_+\sigma_-\,,\boldsymbol{\rho}_t\right] + \Gamma_t\left(\left[\sigma_-\boldsymbol{\rho}_t\,,\sigma_+\right] + \left[\sigma_-\,,\boldsymbol{\rho}_t\sigma_+\right]\right)$$



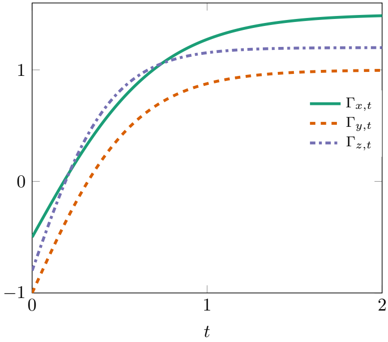


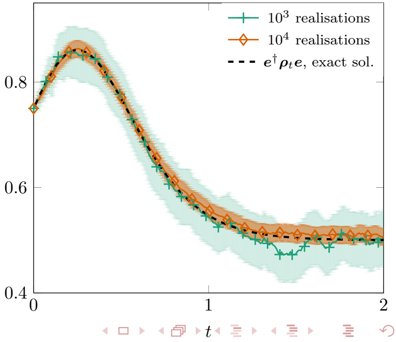
Non positive divisible dynamics

Master equation with negative definite eigenvalue of the rate operator

Caiaffa, Smirne, and Bassi, *Physical Review A*, (2017)

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\rho}_t = \sum_{i=x,y,z} \Gamma_{i,t}(\sigma_i \boldsymbol{\rho}_t \sigma_i - \boldsymbol{\rho}_t)$$





Redfield equation

two non-interacting qubits in contact with the same zero temperature bath

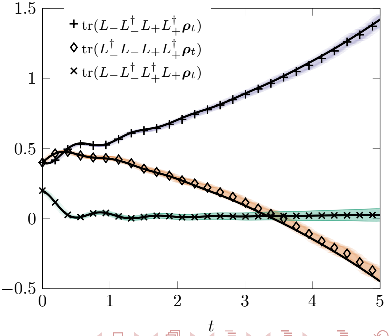
$$\mathrm{H} = \omega_1 \sigma_+ \sigma_- + \omega_2 \tilde{\sigma}_+ \sigma_- + \sum_k \left(\omega_k b_k^\dagger b_k + g_k (\sigma_+ b_k + b_k^\dagger \sigma_-) + \tilde{g}_k (\tilde{\sigma}_+ b_k + b_k^\dagger \tilde{\sigma}_-) \right)$$

Redfield equation does not preserve the positivity of the state operator.

$$\dot{\boldsymbol{\rho}}_t = -\imath\, [\mathrm{H} + \mathrm{S}, \boldsymbol{\rho}_t] + \sum_{\ell = \pm} \lambda_\ell \left(\mathrm{L}_\ell\, \boldsymbol{\rho}_t\, \mathrm{L}_\ell^\dagger - \frac{\mathrm{L}_\ell^\dagger\, \mathrm{L}_\ell\, \boldsymbol{\rho}_t + \boldsymbol{\rho}_t\, \mathrm{L}_\ell^\dagger\, \mathrm{L}_\ell}{2} \right)$$

with

$$\lambda_+ \geq 0 \qquad \& \qquad \lambda_- \leq 0$$



Unraveling of calorimetric measurement

"Hybrid" state operator

$$\boldsymbol{\sigma}_t(\jmath) = \mathrm{Tr}_E\left(e^{-\jmath\,\mathrm{H_E}} e^{-\imath\,H\,t} \frac{e^{-\beta\,\mathrm{H}_E}}{Z} \otimes \boldsymbol{\rho}_0\, e^{\imath\,H\,t} \right)$$

Central fermion model

$$\mathbb{H} = \omega\,\mathrm{a}^{\dagger}\,\mathrm{a} + \sum_{k=1}^{\mathcal{N}} E_k\,\mathrm{c}_k^{\dagger}\,\mathrm{c}_k + \sum_{k=1}^{\mathcal{N}} \left(\bar{g}_k\,\mathrm{a}\,\mathrm{c}_k^{\dagger} + g_k\,\mathrm{c}_k\,\mathrm{a}^{\dagger} \right)$$

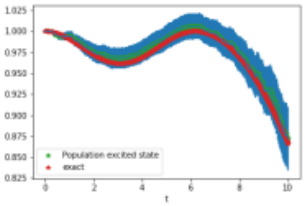
Exact master equation generating a **completely bounded dynamics**

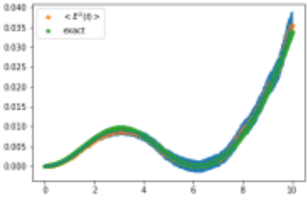
Unraveling with an effective energy exchange process

Unraveling Ansatz

$$\boldsymbol{\sigma}_t = \mathrm{E}\left(e^{-\jmath \epsilon_t}\,\mu_t\,\boldsymbol{\psi}_t \boldsymbol{\psi}_t^{\dagger}\right)$$

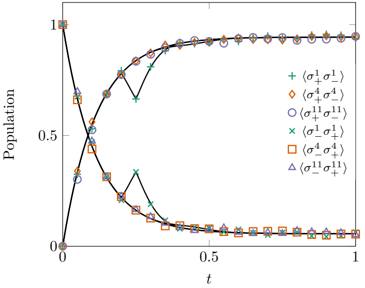
Derive the dynamics of ψ_t AND ϵ_t

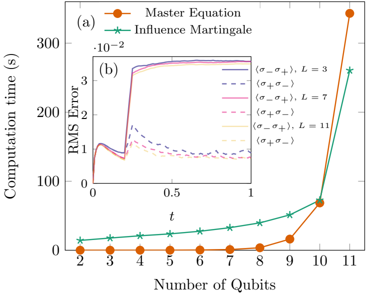




Evolution at zero temperature: model problem $1+1$ fermion

Systems with many degrees of freedom: qubits with non-positive dynamics





Population of sites 1, 4 and 11 of a qubit chain of $L = 11$ elements. The marks show the result of the stochastic evolution and the full black lines the result of numerically integrating the master equation. Only the first qubit has non-positive weight.

(a) Computation time for both the Master Equation and Influence Martingale method as a function of the amount of qubits in the chain. For the stochastic method we generated 1300 realizations. (b) The root mean square error of the populations averaged over all individual sites.

Conclusions and outlook

- Quantum trajectory theory for completely bounded dynamics: master equations beyond weak coupling theory e.g. Redfield equation.
- Thermodynamics beyond weak coupling: influence martingale models heat flow from and to the system.
- Existence of generalized fluctuation relations.
- Applications to state retrodiction and to parameter estimation (compatibility domain problem!).
- Numerical applications: what is the optimal choice of the Poisson rates to generate ostensible distributions?

THANKS!