Time (non)-local Descriptions of Open Quantum System Dynamics

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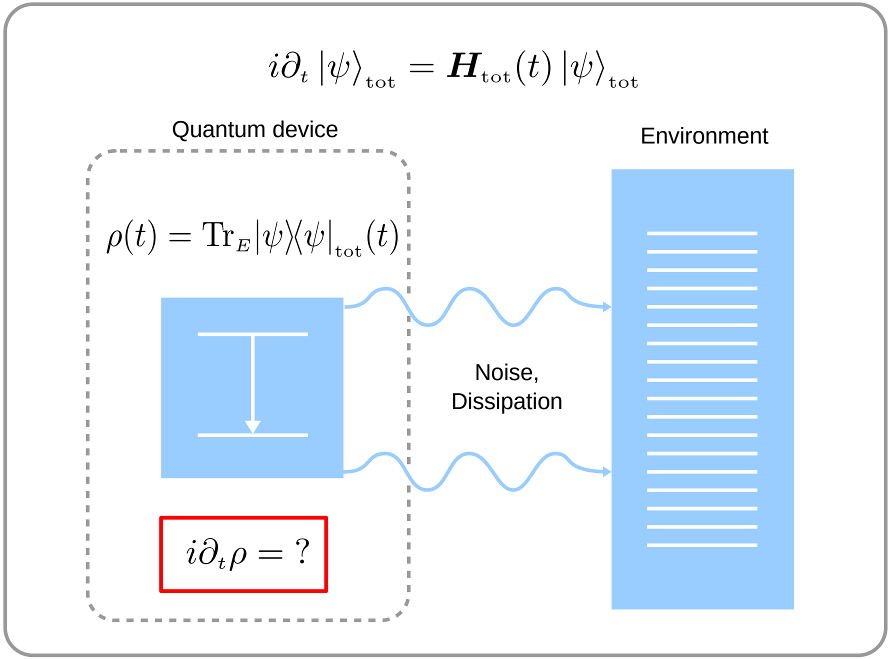
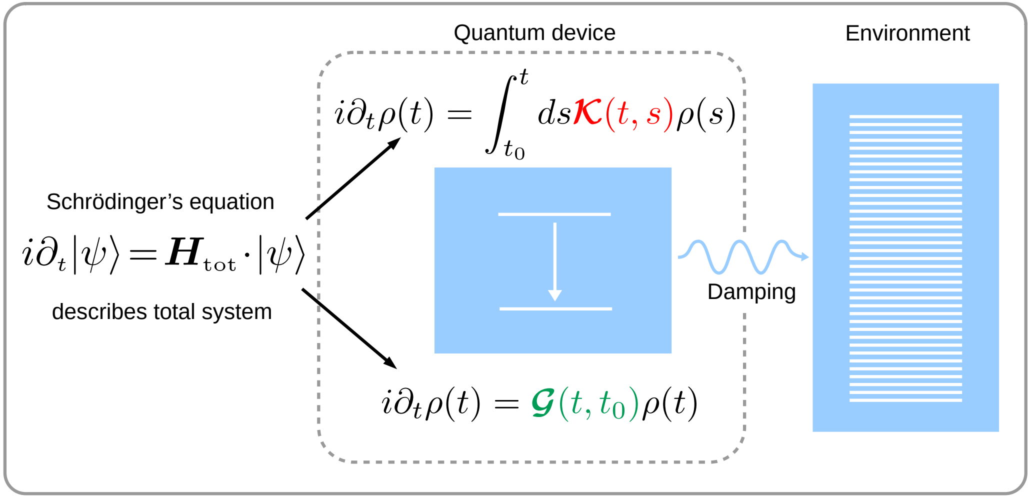
Table of contents

1 Introduction – Dynamical equations of a quantum system



$$|\psi(t)\rangle_{\text{tot}} = U_{\text{tot}}(t, t_0)\, |\psi_0\rangle_{\text{tot}} \quad \xrightarrow[\text{Tr}_E]{?} \quad \rho(t) = \Pi(t, t_0)\, \rho_0$$

1 Introduction – Dynamical equations of a quantum system



"Every theoretical physicist who is any good knows 6 or 7 different theoretical representations for exactly the same physics."

– R. P. Feynman, The character of physical law

1.1 The time-nonlocal approach: microscopic computation, frequency dependence, etc.

$$\boxed{\frac{\partial}{\partial t}\Pi(t,t_0) = -i\int_{t_0}^{t} ds\,\mathcal{K}(t,s)\,\Pi(s,t_0)} \quad \text{where} \quad \rho(t) = \Pi(t,t_0)\,\rho_0$$

1. **'Memory'** as *delayed* backaction of microscopic environment

2. **Frequency domain** for $\mathcal{K}(t,s) = \mathcal{K}(t-s)$

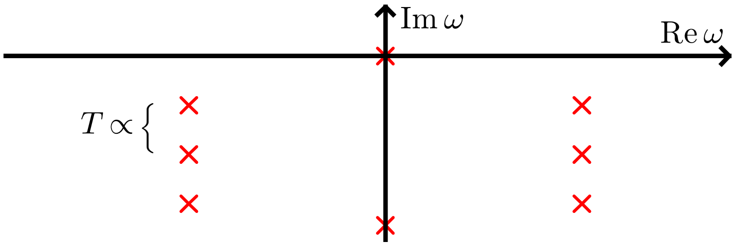
$$\hat{\Pi}(\omega) = \int_0^\infty dt\,\Pi(t)\,e^{i\omega t} = \frac{i}{\omega - \hat{\mathcal{K}}(\omega)}$$

$\Pi(t)$ determined by

→ Poles of $\hat{\Pi}(\omega)$ ⟺ Fixed points $\hat{\mathcal{K}}(\omega_p) = \omega_p$

→ Branch points of $\hat{\Pi}(\omega)$ ⟺ Branch points $\hat{\mathcal{K}}(\omega_p)$

H. Schoeller, Dynamics of open quantum systems, arXiv:1802.10014



3. **Semigroup-Markov approximation:**

$$\dot{\rho}(t) \approx -i\int_{-\infty}^{t} ds\,\mathcal{K}(t-s)\,\rho(t) = -i\,\hat{\mathcal{K}}(0)\,\rho(t)$$

1.2 The time-local approach: complete positivity, quantum Markovianity, etc.

1. **Weakly coupled** system and environment $\Longrightarrow$ dynamics approximated by Lindblad semigroup $\Pi = e^{-i(t-t_0)\mathcal{L}}$

$$\frac{\partial}{\partial t}\Pi(t-t_0) \;=\; -i\,\mathcal{L}\cdot\Pi(t-t_0), \qquad\qquad -i\,\mathcal{L}\,\rho \;=\; -i\,[H\,,\,\rho] + \sum_k \boldsymbol{j_k}\Big[J_k\,\rho\,J_k^\dagger - \tfrac{1}{2}\{J_k^\dagger\,J_k,\,\rho\}\Big]$$

$\rightarrow$ Dynamics is physical (completely positive) iff $j_k \geqslant 0$!

$\rightarrow$ Often phenomenological construction of J_k

1.2 The time-local approach: complete positivity, quantum Markovianity, etc.

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→ Often phenomenological construction of J_k

2. **Strongly coupled** system and environment $\Longrightarrow$ Every dynamics admits time-local QME *by construction*

Define[1] $\mathcal{G} := i\,\dot{\Pi}\,\Pi^{-1} \quad \Longrightarrow \quad \frac{\partial}{\partial t}\Pi(t,t_0) = -i\,\mathcal{G}(t,t_0)\,\Pi(t,t_0)$

$$-i\,\mathcal{G}(t,t_0)\,\rho = -i\,[H(t,t_0),\rho] + \sum_k \boldsymbol{j_k(t,t_0)}\Big[J_k(t,t_0)\,\rho\,J_k^\dagger(t,t_0) - \tfrac{1}{2}\{J_k^\dagger(t,t_0)\,J_k(t,t_0),\rho\}\Big]$$

→ Physical generators with $j_k(t,t_0) < 0$ possible...

"Weakly Markovian" (divisible) iff $j_k(t,t_0) \geqslant 0$

→ Necessary to derive $\mathcal{G}$ from total Hamiltonian $H_{\text{tot}} = H + H_R + H_I$

3. **Semigroup-Markov approximation:**

$$\mathcal{L} = \lim_{t_0\to-\infty}\mathcal{G}(t-t_0) = \mathcal{G}(\infty) \qquad \mathcal{G}(\infty) \overset{?}{=} \hat{\mathcal{K}}(0)$$

1. What if Π is not invertible ?

2 The fixed-point relation

What is the explicit relation between $\mathcal{K}$ and $\mathcal{G}$?

Why bother ?

Two fundamental QMEs offer mutually exclusive insights into the solution:

- $\mathcal{K}$ better: microscopic pictures, sophisticated approximation schemes, renormalization groups, ...
- $\mathcal{G}$ better: quantum information, Markovianity, stochastic simulations, ...

2 The fixed-point relation

What is the explicit relation between $\mathcal{K}$ and $\mathcal{G}$?

Recall Laplace transform of $\mathcal{K}$:

$$\hat{\mathcal{K}}(\omega) \;=\; \int_{-\infty}^{t} \mathrm{d}s\, \mathcal{K}(t-s)\, e^{i\,(t-s)\,\omega}$$

Define functional generalization:

$$\hat{\mathcal{K}}[X(\tau)](t,t_0) \;=\; \int_{t_0}^{t} \mathrm{d}s\, \mathcal{K}(t,s)\, \mathcal{T}_{\rightarrow}\, e^{i\int_s^t \mathrm{d}\tau X(\tau)}$$

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The generator $\mathcal{G}$ is a *fixed point* of this functional[2]:

$$\boxed{\mathcal{G}(t,t_0) \;=\; \hat{\mathcal{K}}[\mathcal{G}](t,t_0)}$$

2. Phys. Rev. X **11**, 021041 (Nestmann, Bruch, Wegewijs 2021)

2.1 Translation of perturbative series

- **Idea:** $\mathcal{K}$ has the simplest building-blocks

  $\rightarrow$ use $\mathcal{G} = \hat{\mathcal{K}}[\mathcal{G}](t, t_0)$ to translate series expansion from $\mathcal{K}$ to $\mathcal{G}$ (around bare Liouvillian $\mathcal{L} = [H, \bullet]$)

  $\mathcal{G}_{\text{aprx}} = \mathcal{L} + \mathcal{G}^{(2)} + \mathcal{G}^{(4)}$ will give a different approximation than $\mathcal{K}_{\text{aprx}} = \mathcal{L}\,\delta + \mathcal{K}^{(2)} + \mathcal{K}^{(4)}$!

- **General result:** $\mathcal{G}$ admits recursive expansion[3]

$$\mathcal{G}(t) = \mathcal{L} + \mathcal{G}^{(2)} + \mathcal{G}^{(4)} + \cdots \stackrel{!}{=} \hat{\mathcal{K}}[\mathcal{G}](t) = \mathcal{L} + \int_{t_0}^{t} \mathrm{d}s \left[\mathcal{K}^{(2)}(t,s) + \mathcal{K}^{(4)}(t,s) + \cdots\right] \mathcal{T}_{\rightarrow} e^{i\int_s^t \mathrm{d}\tau\, (\mathcal{L} + \mathcal{G}^{(2)}(\tau) + \mathcal{G}^{(4)}(\tau) + \cdots)}$$

- **Organize order-by-order:**

$$\mathcal{G}^{(2)}(t, t_0) = \int_{t_0}^{t} \mathrm{d}s\, \mathcal{K}^{(2)}(t,s)\, e^{i\mathcal{L}(t-s)}$$

$$\mathcal{G}^{(4)}(t, t_0) = \int_{t_0}^{t} \mathrm{d}s\, \mathcal{K}^{(4)}(t,s)\, e^{i\mathcal{L}(t-s)} + i \int_{t_0}^{t} \mathrm{d}s \int_{s}^{t} \mathrm{d}\tau\, \mathcal{K}^{(2)}(t,s)\, e^{i\mathcal{L}(\tau - s)}\, \mathcal{G}^{(2)}(\tau, t_0)\, e^{i\mathcal{L}(t-\tau)}$$

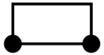
3. Phys. Rev. B 104, 155407 (Nestmann, Wegewijs 2021)

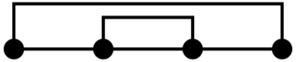
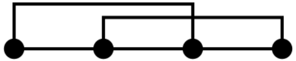
Example: Anderson quantum dot

Simplest model of tunneling through a quantum dot:

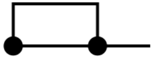
$$H_{\mathrm{tot}} \;=\; \varepsilon\,(n_\uparrow + n_\downarrow) + U\,n_\uparrow\,n_\downarrow + \sum_{r,\sigma} \int \mathrm{d}\omega\,(\omega + \mu_r)\,a^\dagger_{r\sigma}(\omega)\,a_{r\sigma}(\omega) + \sum_{r,\sigma} \sqrt{\frac{\Gamma}{2\pi}} \int \mathrm{d}\omega\,\Big(a^\dagger_{r\sigma}(\omega)\,d_\sigma + d^\dagger_\sigma\,a_{r\sigma}(\omega)\Big)$$

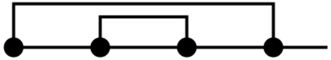
Real-time diagrammatic expansion of $\mathcal{K}$:[4]

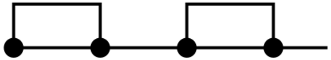
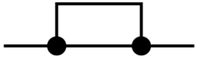
$-i\mathcal{K}^{(2)} =$ 

$-i\mathcal{K}^{(4)} =$  $+$ 

Translated diagrammatic expansion for $\mathcal{G}$:

$-i\mathcal{G}^{(2)} =$  $\cdot\Pi_0^\dagger$

$-i\mathcal{G}^{(4)} =$  $\cdot\Pi_0^\dagger$ $+$  $\cdot\Pi_0^\dagger$

$+$  $\cdot\Pi_0^\dagger$ $-$  $\cdot\Pi_0^\dagger\cdot$  $\cdot\Pi_0^\dagger$

4. Eur. Phys. J. Special Topics 168, 179-266 (Schoeller, 2009), Phys. Rev. B 90, 045407 (Saptsov, Wegewijs 2014)

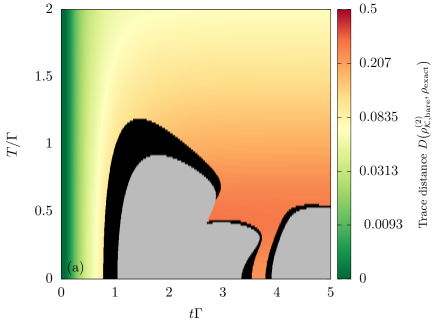
Example: Anderson quantum dot ($U = 0$)

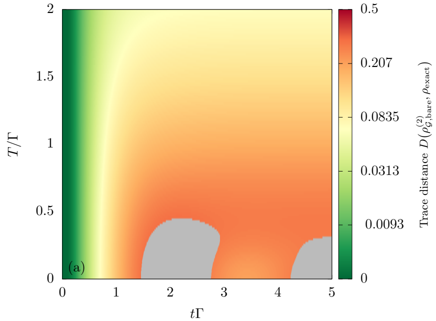
Order

$\mathcal{K}(s)$

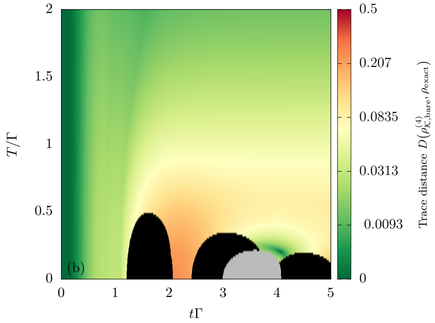
$\mathcal{G}(t)$

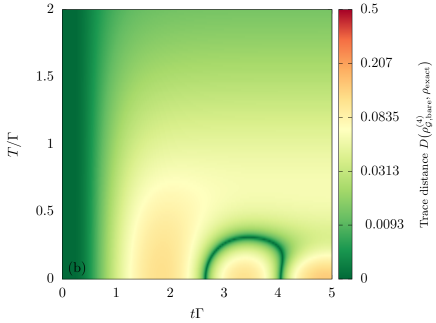
2





4





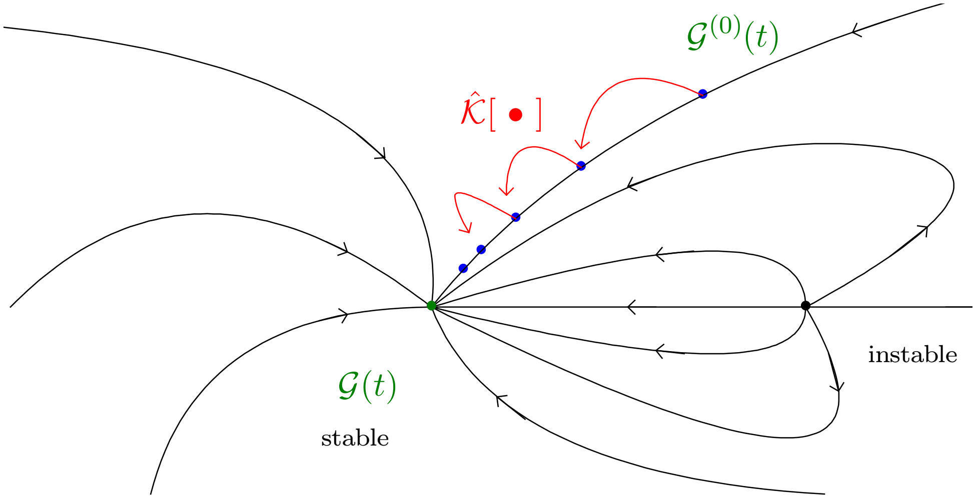
2.2 Iterative calculation of generator from memory kernel

$$\mathcal{G}_{\text{it}}^{(n+1)}(t,t_0) \;:=\; \hat{\mathcal{K}}[\mathcal{G}_{\text{it}}^{(n)}](t,t_0)$$

1. Convenient initial guess
   - Markovian: $\mathcal{G}^{(0)} = \hat{\mathcal{K}}(0)$ or $\mathcal{G}(\infty)$
   - Redfield: $\mathcal{G}^{(0)}(t) = \int_{t_0}^{t} \mathrm{d}s\, \mathcal{K}(s)$
2. Iterate:

$$\mathcal{G}(t) = \hat{\mathcal{K}}\Big[\ldots\hat{\mathcal{K}}[\hat{\mathcal{K}}[\mathcal{G}^{(0)}]]\Big]$$

3. It converges !



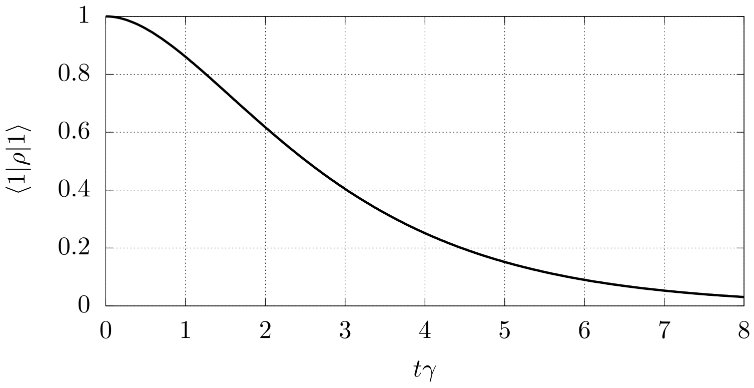
Space of superoperator functions of time

Atomic damping: physical singularities of the generator !

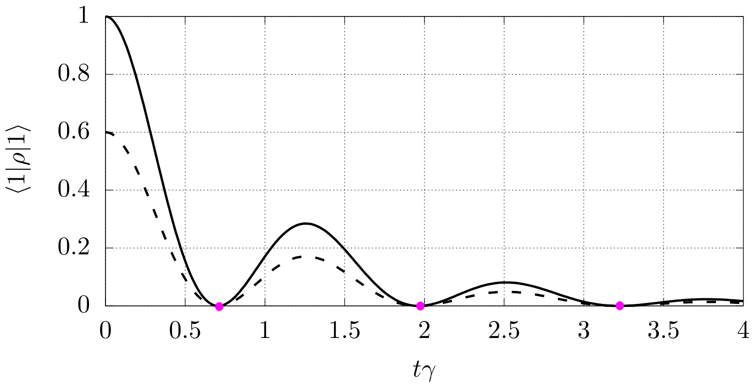
- Dissipative Jaynes-Cummings model with $\Gamma(\omega) = \Gamma \cdot \frac{\gamma^2}{\gamma^2 + (\omega - \varepsilon)^2}$
  Garraway, Phys. Rev. A **55**, 2290 (1997)

$$H + H_E + H_I = \varepsilon d^\dagger d + \int d\omega \omega b_\omega^\dagger b_\omega + \int d\omega \sqrt{\frac{\Gamma(\omega)}{2\pi}} (d^\dagger b_\omega + b_\omega^\dagger d), \qquad \rho_R = |0\rangle\langle 0|$$

overdamped regime ($\gamma \geqslant 2\,\Gamma$)

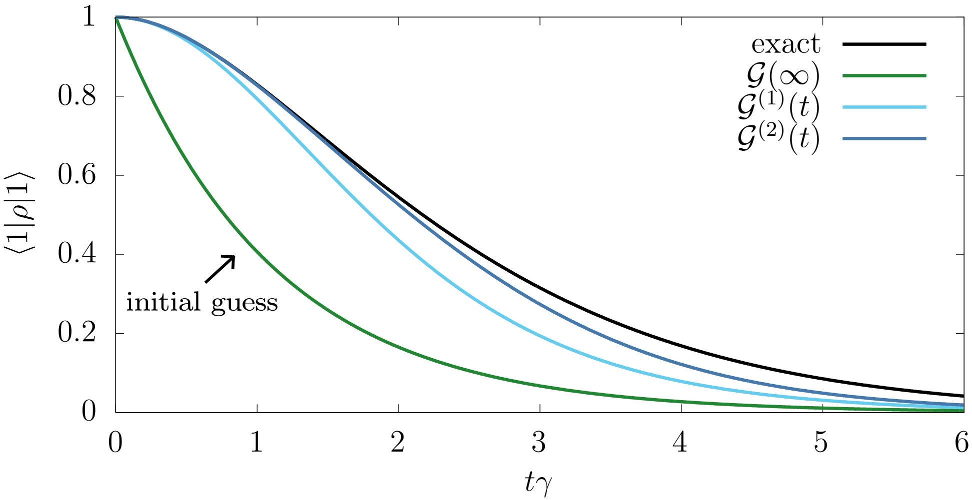


underdamped regime ($\gamma < 2\,\Gamma$)



- Perturbation theory limited by first singularity in time Breuer, Kappler, Petruccione, Phys. Rev. A **59**, 1633 (1999)

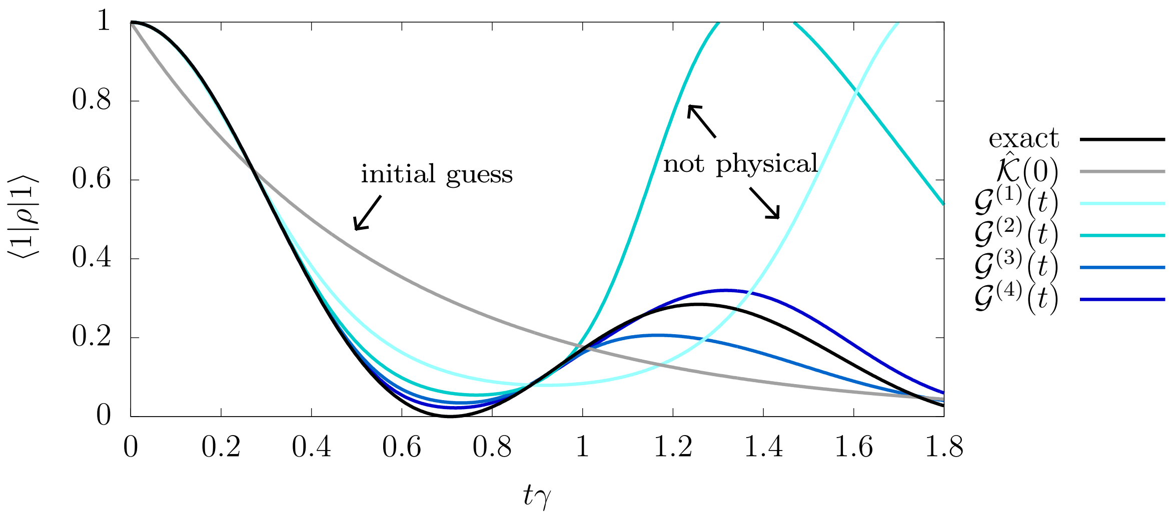
Example: overdamped Jaynes-Cummings model



Convergence in n is 'uniform' in time:

- Small times: correct curvature guaranteed
- Large times: correct stationary limit guaranteed for each iteration n for appropriate starting points like $\mathcal{G}(\infty)$

Example: underdamped Jaynes-Cummings model



- Works *beyond* singularity in underdamped regime (unlike perturbation theory) !
- Construct $\mathcal{G}(t)$ from $\mathcal{K}(t)$ which produces *same* solution

3 The stationary generator: non-perturbative Markov approximations

Using the simpler functional

$$\hat{\mathcal{K}}(X) := \int_0^\infty \mathrm{d}t\, \mathcal{K}(t)\, e^{itX}$$

the stationary generator $\mathcal{G}(\infty)$ is also a fixed point:

$$\boxed{\mathcal{G}(\infty) = \hat{\mathcal{K}}(\mathcal{G}(\infty))}$$

Immediate insights:

→ $\mathcal{G}(\infty)$ and $\hat{\mathcal{K}}(0)$ have exact same stationary state[5]: $\mathcal{G}(\infty)\,\rho_\infty = 0 = \hat{\mathcal{K}}(0)\,\rho_\infty$

→ There is no unique (non-perturbative) Markov approximation: $\mathcal{G}(\infty) \neq \hat{\mathcal{K}}(0)$

→ Spectrum of $\mathcal{G}(\infty)$ completely determined from $\hat{\mathcal{K}}(\omega)$

5. Careful: not true for perturbative approximations of $\mathcal{G}(\infty)$ and $\hat{\mathcal{K}}(0)$!

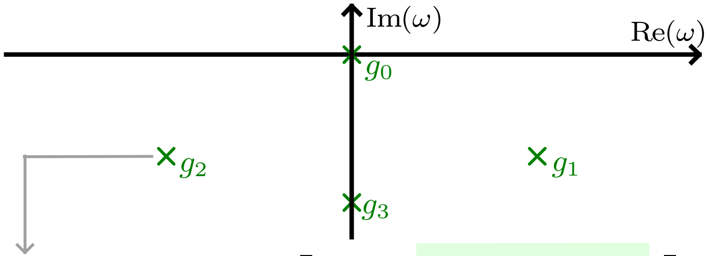
3.1 The stationary generator: finite-frequency sampling

$$\mathcal{G}(\infty) \;=\; \int_0^\infty \mathrm{d}t\, \mathcal{K}(t)\, e^{it\mathcal{G}(\infty)}$$

Act with right eigenvector $|g_i)$ on $\mathcal{G}(\infty)$:

$$g_i\,|g_i) \;=\; \int_0^\infty \mathrm{d}t\, \mathcal{K}(t)\, e^{itg_i}\,|g_i) \;=\; \hat{\mathcal{K}}(g_i)\,|g_i)$$

$\rightarrow$ Eigenvalues g_i are fixed points of $\hat{\mathcal{K}}$ $\iff$ g_i are poles of $\hat{\Pi}(\omega) = \frac{i}{\omega - \hat{\mathcal{K}}(\omega)}$!

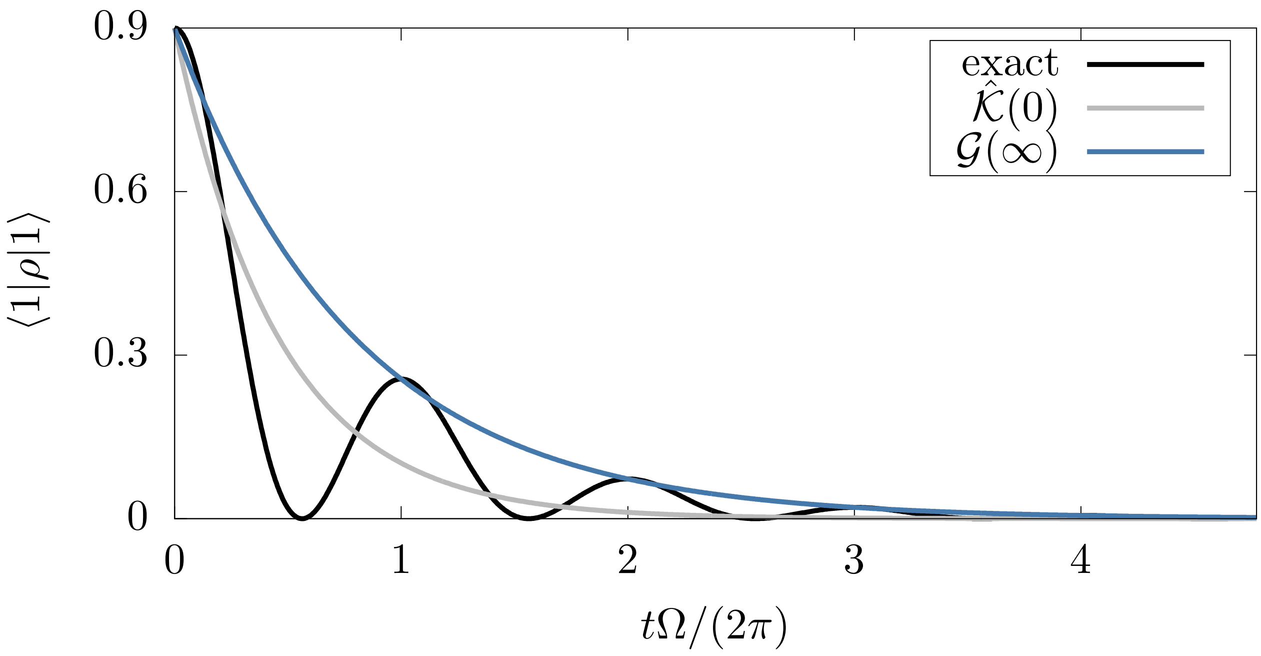


$\mathcal{G}(\infty)$ samples $\hat{\mathcal{K}}(\omega)$ at pole-frequencies of $\hat{\Pi}(\omega)$.

$$\hat{\mathcal{K}}(g_2) = k_0(g_2)\,|k_0(g_2))(\bar{k}_0(g_2)| + \underbrace{\boldsymbol{k_1(g_2)}}_{= \boldsymbol{g_2}}\,\underbrace{|\boldsymbol{k_1(g_2))}}_{= |\boldsymbol{g_2})}(\bar{k}_1(g_2)| + \cdots$$

$\rightarrow$ Main difference between $\mathcal{G}(\infty)$ and $\hat{\mathcal{K}}(0)$: $\mathcal{G}(\infty)$ knows about most important (?) decay rates

Example: Jaynes-Cummings model



3.2 Perturbative expansion of stationary generator

Expand stationary fixed-point equation (time-translation invariant systems):

$$\mathcal{G}(\infty) \;=\; \mathcal{L} + \mathcal{G}^{(2)}(\infty) + \cdots \;\stackrel{!}{=}\; \hat{\mathcal{K}}(\mathcal{G}(\infty)) \;=\; \mathcal{L} + \int_0^t \mathrm{d}s \left[\mathcal{K}^{(2)}(t-s) + \mathcal{K}^{(4)}(t-s) + \cdots\right] e^{i(\mathcal{L}+\mathcal{G}^{(2)}(\infty)+\cdots)(t-s)}$$

Interaction picture:

$$\mathcal{G}_I^{(2)}(\infty) \;=\; \hat{\mathcal{K}}_I^{(2)}(0), \qquad \mathcal{G}_I^{(4)}(\infty) \;=\; \hat{\mathcal{K}}_I^{(4)}(0) + \frac{\partial \hat{\mathcal{K}}_I^{(2)}}{\partial \omega}(0)\, \hat{\mathcal{K}}_I^{(2)}(0)$$

Schrödinger picture: using supervector notation $|kl) := |k\rangle\langle l|$ with $\mathcal{L}|kl) = (E_k - E_l)\,|kl) = \Delta_{kl}\,|kl)$:

$$\mathcal{G}^{(2)}(\infty) \;=\; \sum_{kl} \hat{\mathcal{K}}^{(2)}(\Delta_{kl})\,|kl)(kl|$$

$$\mathcal{G}^{(4)}(\infty) \;=\; \sum_{kl} \hat{\mathcal{K}}^{(4)}(\Delta_{kl})\,|kl)(kl| + \sum_{kl,k'l'} \delta\hat{\mathcal{K}}^{(2)}(\Delta_{kl},\Delta_{k'l'})\,|kl)(kl|\mathcal{G}^{(2)}(\infty)|k'l')(k'l'|$$

$$\text{where } \delta\hat{\mathcal{K}}^{(2)}(\Delta_{kl},\Delta_{k'l'}) = \begin{cases} \frac{\partial \hat{\mathcal{K}}^{(2)}}{\partial \omega}(\Delta_{kl}) & \text{if } \;\Delta_{kl} = \Delta_{k'l'} \\ \frac{\hat{\mathcal{K}}^{(2)}(\Delta_{kl}) - \hat{\mathcal{K}}^{(2)}(\Delta_{k'l'})}{\Delta_{kl} - \Delta_{k'l'}} & \text{otherwise} \end{cases}$$

Thank you for your attention

Summary: There exist two approaches to open system dynamics featuring $\mathcal{K}$ and $\mathcal{G}$. These are linked via a functional fixed-point relation $\mathcal{G} = \hat{\mathcal{K}}[\mathcal{G}]$. Simpler building blocks of $\mathcal{K}$ can be used to compute $\mathcal{G}$.

More of my work: konstantin-nestmann.com

- Fixed-point relation $\mathcal{G} = \hat{\mathcal{K}}[\mathcal{G}]$ & transformation of perturbation expansions:
  Nestmann, Bruch, Wegewijs, Phys. Rev. X **11**, 021041 (2021)
  Nestmann, Wegewijs, Phys. Rev. B **104**, 155407 (2021)

- T - flow renormalization group:
  Nestmann and Wegewijs, SciPost Phys. **12**, 121 (2022)

- Channel theory, fermionic duality, quantum (non)-Markovianity:
  Bruch, Nestmann, Schulenborg, Wegewijs, SciPost Phys. **11**, 053 (2021)
  Reimer, Wegewijs, Nestmann and Pletyukhov, J. Chem. Phys. **151**, 044101 (2019)