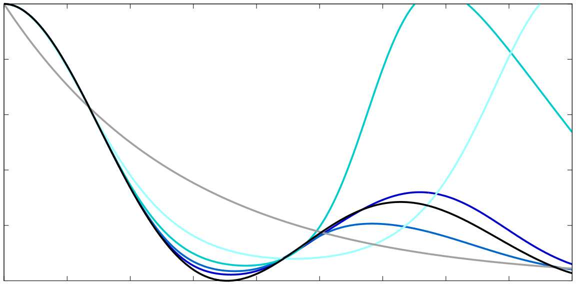
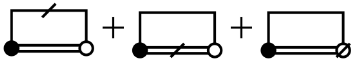
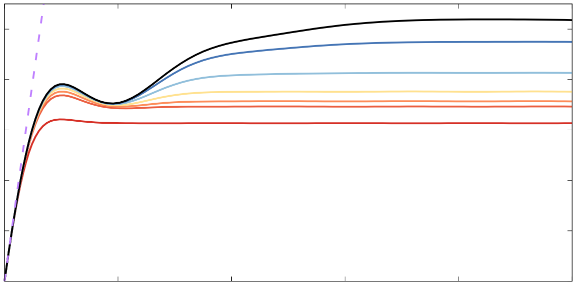
Open Quantum Systems:
Time (non)-locality, Fixed Points, and Renormalization Groups

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



$$-i\frac{\partial \Sigma}{\partial T} =$$

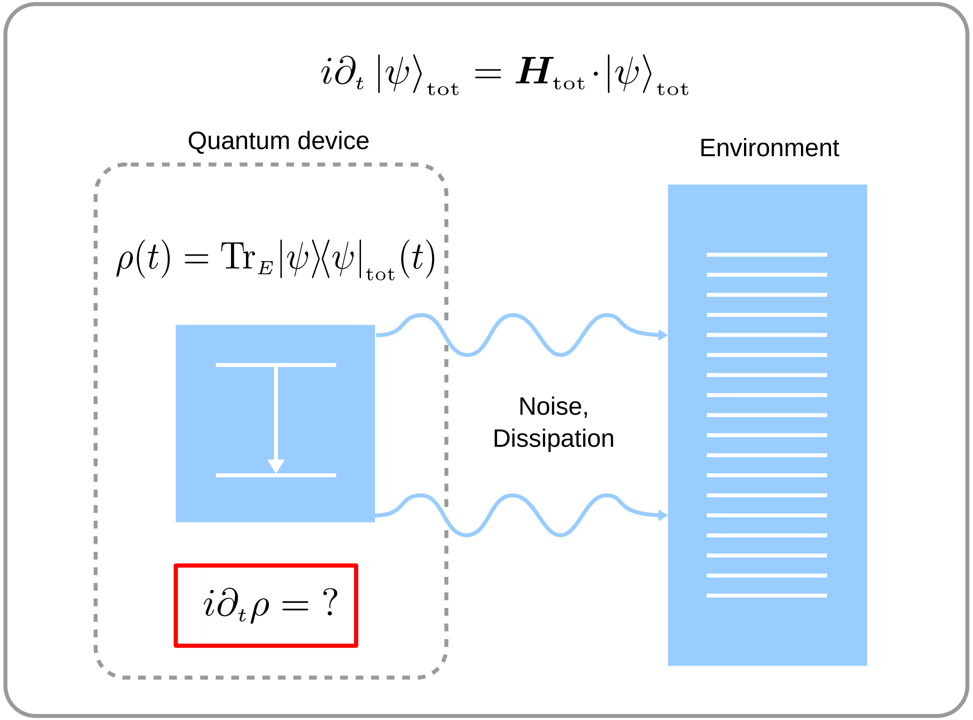




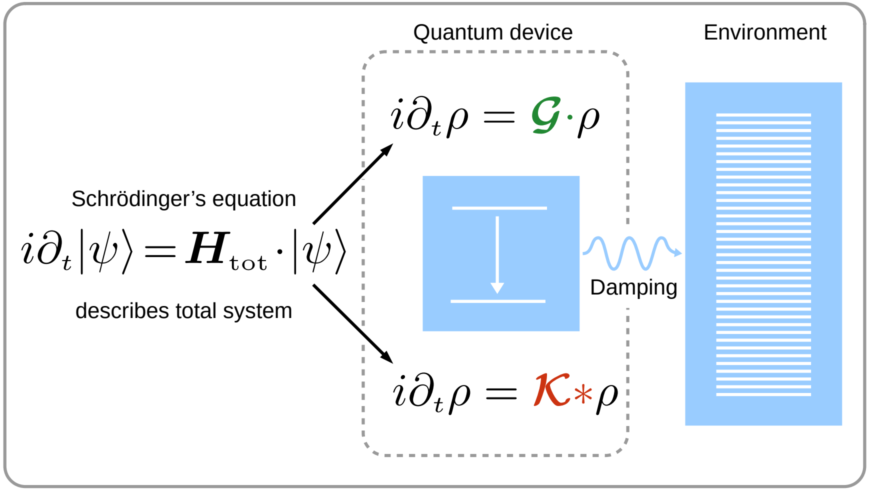
Konstantin Nestmann

Table of contents

1 Introduction – Dynamical equations of a quantum system



1 Introduction – Dynamical equations of a quantum system



2 Why bother ?

If you *already* have a quantum master equation (QME) in hand,
why would you bother to construct *another one* **?**

[R. P. Feynman][1]: "Every theoretical physicist who is any good knows 6 or 7 different theoretical representations for exactly the same physics."

Two fundamental QMEs offer mutually exclusive insights into the solution: $\rho(t) = \Pi(t - t_0)\,\rho(t_0)$

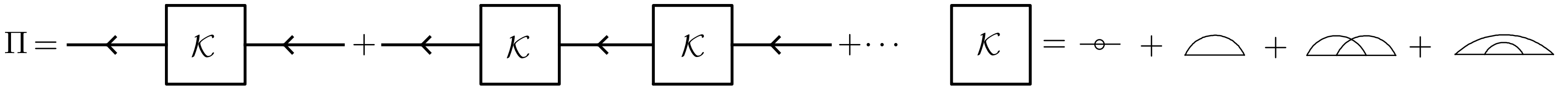
- $\mathcal{K}$ better: microscopic pictures, approximation schemes, renormalization groups, ...
- $\mathcal{G}$ better: Quantum information, Markovianity, stochastic simulations, ...

1. From *The character of physical law.*

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

$$\frac{\partial}{\partial t}\Pi(t,t_0) \;=\; -i\int_{t_0}^{t} \mathrm{d}s\, \mathcal{K}(t,s)\, \Pi(s,t_0)$$

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



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

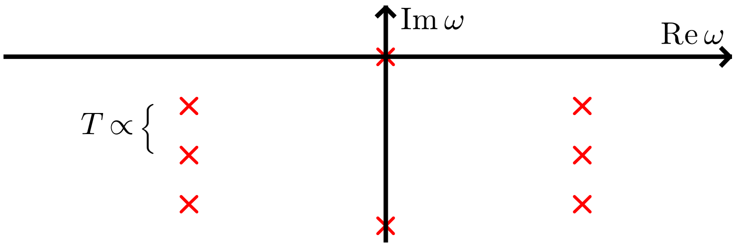
$$\hat{\Pi}(\omega) \;=\; \int_0^\infty \mathrm{d}t\, \Pi(t)\, e^{i\omega t} \;=\; \frac{i}{\omega - \hat{\mathcal{K}}(\omega)}$$

$\Pi(t)$ determined by

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

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

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



3. **Semigroup-Markov approximation:**

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

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

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

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

$\rightarrow$ Completely positive solution guaranteed by $j_k \geqslant 0$!

$\rightarrow$ Phenomenological construction of J_k “can’t go wrong”

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

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

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

$\rightarrow$ Complete positivity but $j_k(t,t_0) < 0$ possible...

Markovianity based on $j_k(t,t_0)$!

$\rightarrow$ Necessary to derive $\mathcal{G}$ from total Hamiltonian $H_{\text{tot}} = H + H_{\text{R}} + H_{\text{T}}$

3. **Semigroup-Markov approximation:**

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

3 The fixed-point relation

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

Construct following functional generalization of the Laplace transform of $\mathcal{K}$

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

$$\text{compare:} \quad \hat{\mathcal{K}}(\omega) \;=\; \int_{-\infty}^{t} \mathrm{d}s\, \mathcal{K}(t-s)\, e^{i(t-s)\omega} \;=\; \int_{0}^{\infty} \mathrm{d}s\, \mathcal{K}(s)\, e^{is\omega}$$

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

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

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

Stationary limit $t_0 \to -\infty$: the functional simplifies, $\lim_{t_0\to-\infty} \hat{\mathcal{K}}[X] = \mathcal{K}(X) = \int_0^\infty \mathrm{d}t\, \mathcal{K}(t)\, e^{itX}$ and $\mathcal{G}(\infty) = \hat{\mathcal{K}}(\mathcal{G}(\infty))$.

Iterative calculation of generator from memory kernel

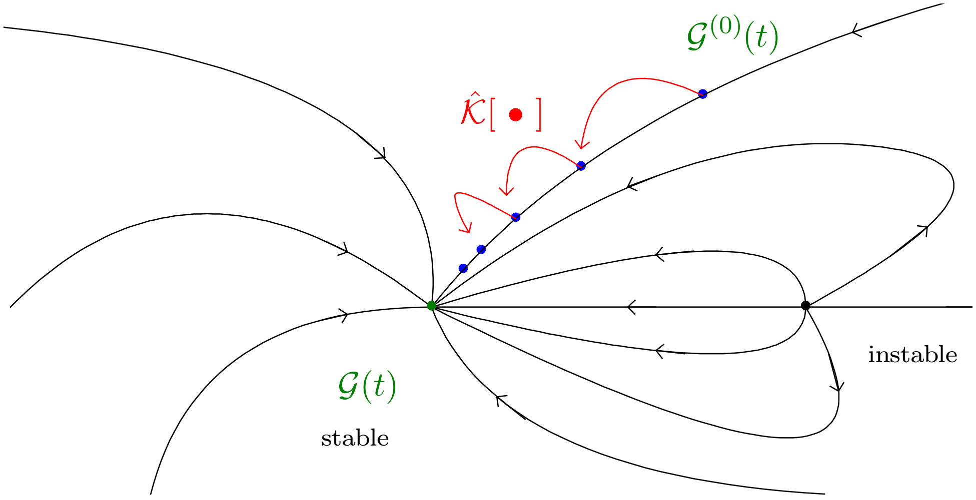
$$\mathcal{G}^{(n+1)}(t,t_0) \;:=\; \hat{\mathcal{K}}[\mathcal{G}^{(n)}](t,t_0)$$

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 !



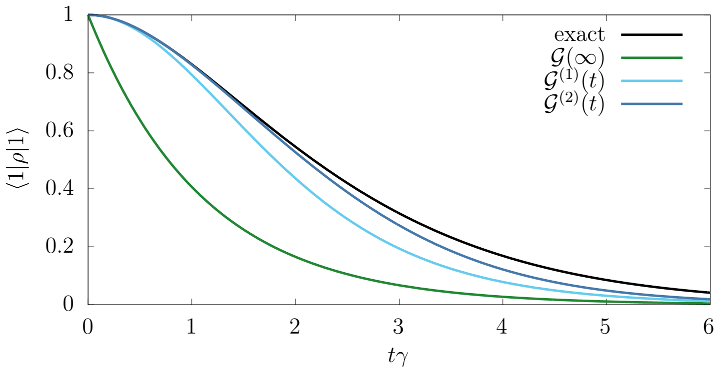
Space of superoperator functions of time

Atomic damping: Physical singularities of the generator !

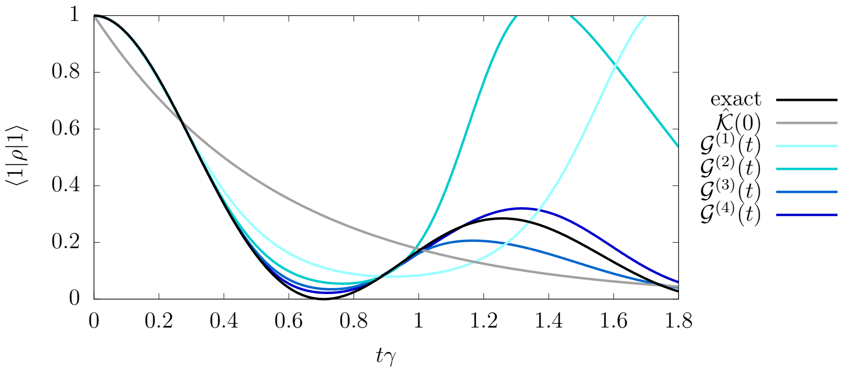
Dissipative Jaynes-Cummings model with $\Gamma(\omega) = \Gamma \cdot \frac{\gamma^2}{\gamma^2 + (\omega - \varepsilon)^2}$ Garraway, Phys. Rev. A **55**, 2290 (1997)

$$H + H_\mathrm{R} + H_\mathrm{T} = \varepsilon d^\dagger d + \int \mathrm{d}\omega \omega b_\omega^\dagger b_\omega + \int \mathrm{d}\omega \sqrt{\frac{\Gamma(\omega)}{2\pi}} (d^\dagger b_\omega + b_\omega^\dagger d), \qquad \rho_\mathrm{R} = |0\rangle\langle 0|$$

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



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



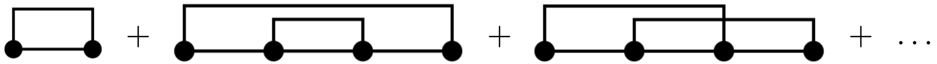
Small times: correct curvature
Large times: correct stationary limit

Works *beyond* singularity (unlike perturbation theory) !

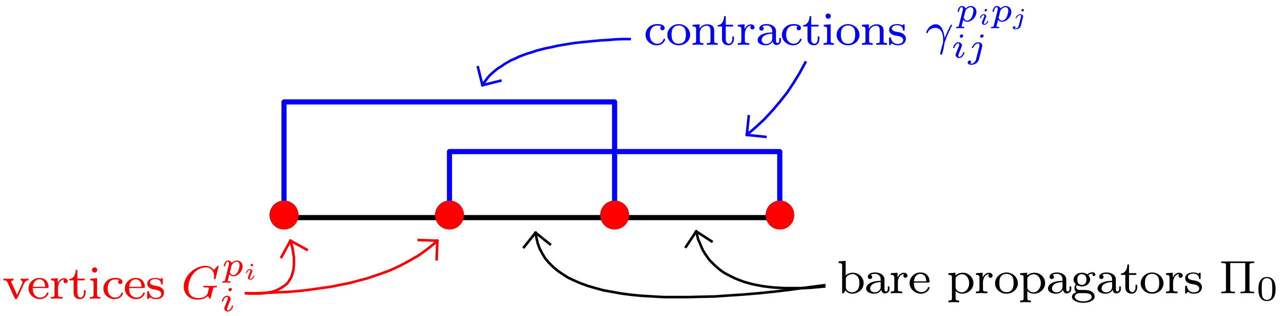
4 Microscopic computations – perturbation theory and beyond

Memory kernel perturbation theory well-developed[2]:

- Time-space and frequency-space formulations (“Real-time diagrammatics”, also in QmeQ)
- Keldysh + superoperator version

$-i\mathcal{K} =$ 

Each diagram consists of three parts:



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2. Schoeller, König Phys. Rev. Lett. 84 (2000), Korb, Reininghaus, Schoeller, König, Phys. Rev. B 76, 165316 (2007)

4.1 Superfermions and renormalized perturbation theory

Instead of defining $G_1^p \bullet = \begin{cases} d_1 \bullet & p=1 \\ \bullet d_1 & p=-1 \end{cases}$ define instead "superfermions"[3] $G_1^p \bullet = \frac{1}{\sqrt{2}}\left(d_1 \bullet + p\,(-\mathbb{1})^n \bullet (-\mathbb{1})^n d_1\right)$

$\Longrightarrow$ Only two non-zero contractions: $\gamma_1^{-+}(t) \propto \delta(t)$ and $\gamma_1^{--}(t)$!

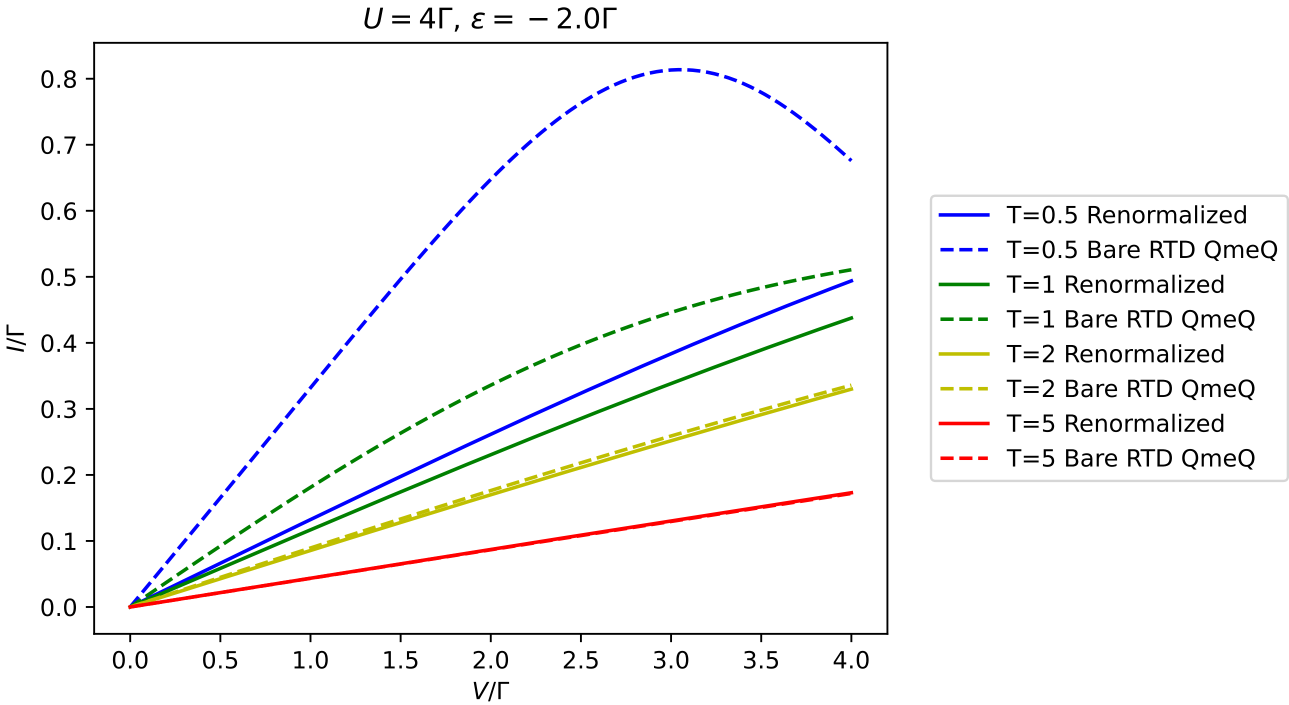
Exactly resum "trivial" $\gamma_1^{-+}(t)$ contractions:

- Replace bare Liouvilloan $L_0 = [H_0, \bullet]$ $\longrightarrow$ $L_\infty = L_0 + \Sigma_\infty$ with infinite temperature Liouvilloan
- Only creation superoperators G_1^+ allowed
- Same diagrams, different translation $\longrightarrow$ cheap improvement bare pert. theory

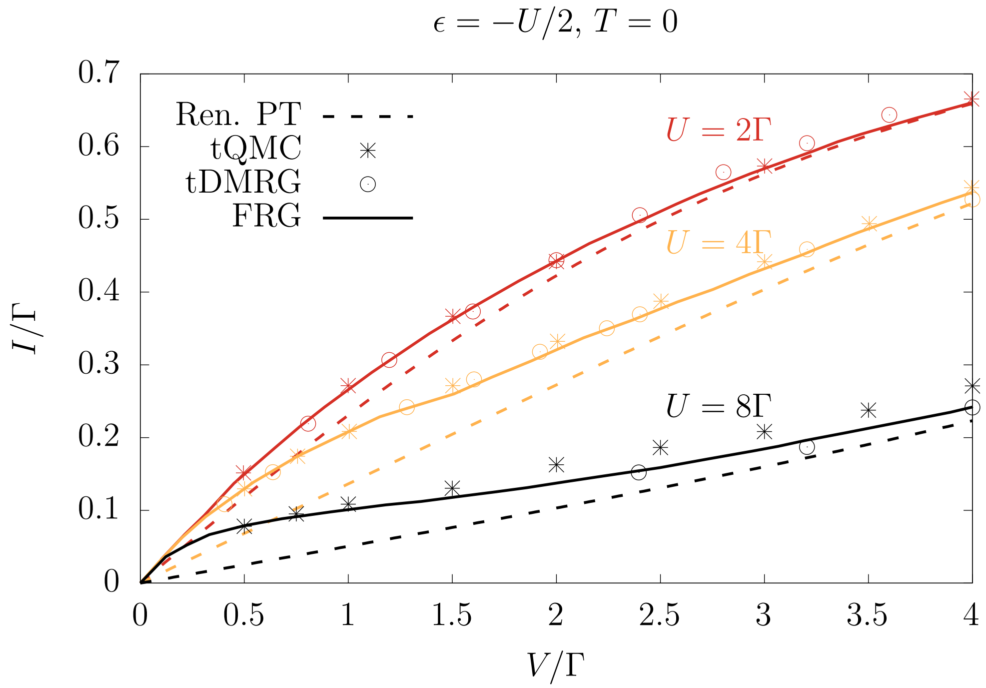
Resulting PT is exact for $\Gamma \to 0$, $T \to \infty$ and terminates for $U = 0$!

3. Saptsov and Wegewijs, Phys. Rev. B 86, 235432 (2012), Saptsov Wegewijs, Phys. Rev. B 90, 045407 (2014)

Benchmark vs bare perturbation theory (RTD QmeQ)



Benchmark vs QMC, DMRG, FRG



Eckel *et al*, New J. Phys. **12**, 043042 (2010), Werner *et al*, Phys. Rev. B **81**, 035108 (2010)

4.2 T - flow renormalization group

Inspired by Wilson's RG:[4]

- Perturbative descriptions fail whenever systems lack characteristic scale:
  - Magnet at critical point → magnetization fluctuates with all wavelengths → missing length scale
  - QED → intermediate states with arbitrary magnitude momentum → missing energy scale
- Replace Hamiltonian H with simpler effective Hamiltonian H_N and $H = \lim_{N\to\infty} H_N$
- Use RG transformation $H_{N+1} = \mathcal{F}[H_N]$
- Each step $H_N \to H_{N+1}$ represents small perturbation → compute systematically

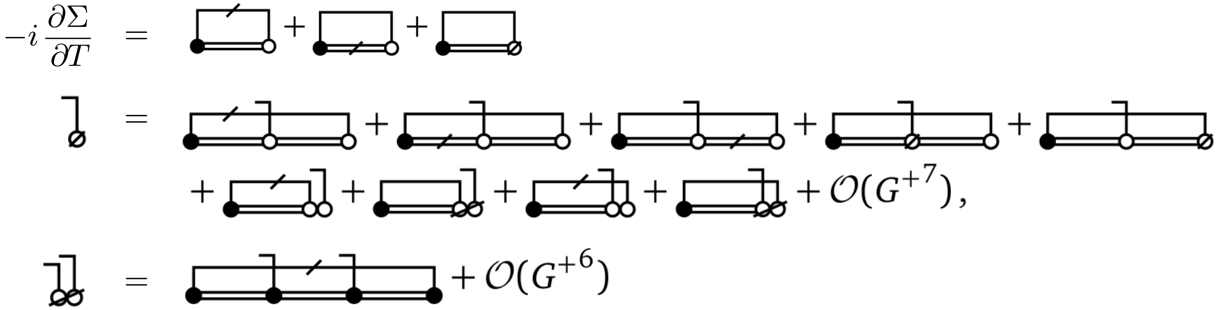
Idea T-flow [technical inspiration "E-flow"[5]]:

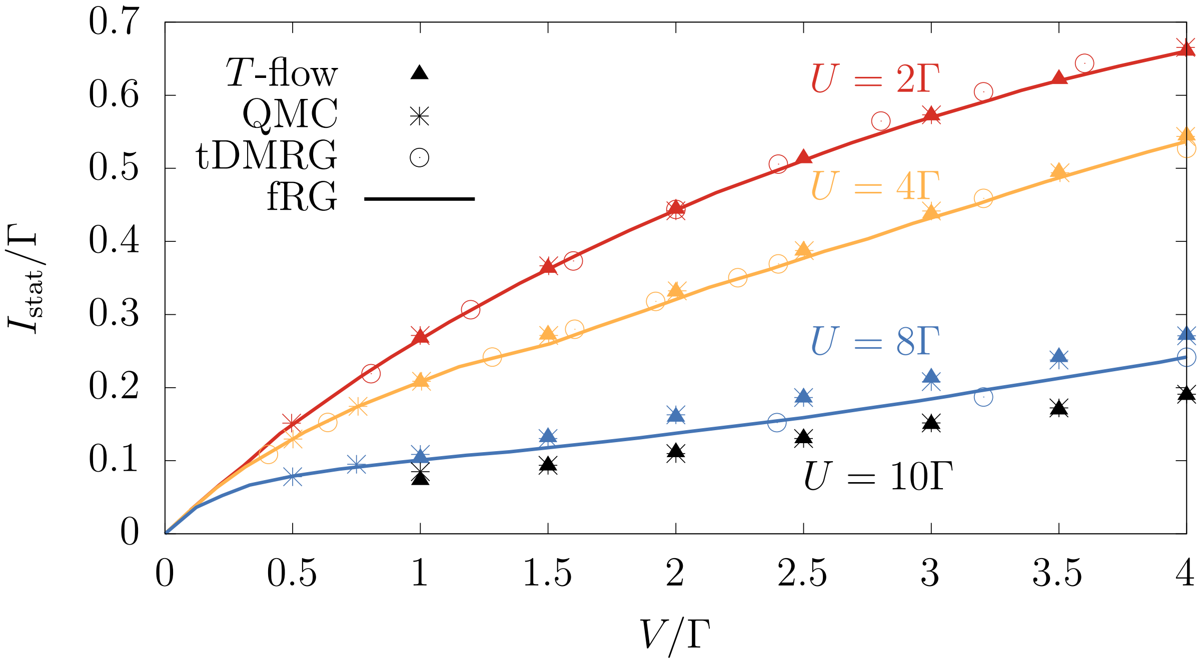
- Temperature sets the inverse correlation time reservoirs
- Use RG transformation $\mathcal{K}_{T-\delta T} = \mathcal{F}[\mathcal{K}_T]$
- Lower T in small steps $\longrightarrow$ increase effective coupling

4. Wilson Rev. Mod. Phys. 47, 773–840 (1975)
5. Pletyukhov and Schoeller, Phys. Rev. Lett. 108, 260601 (2012)

Derive RG equations:

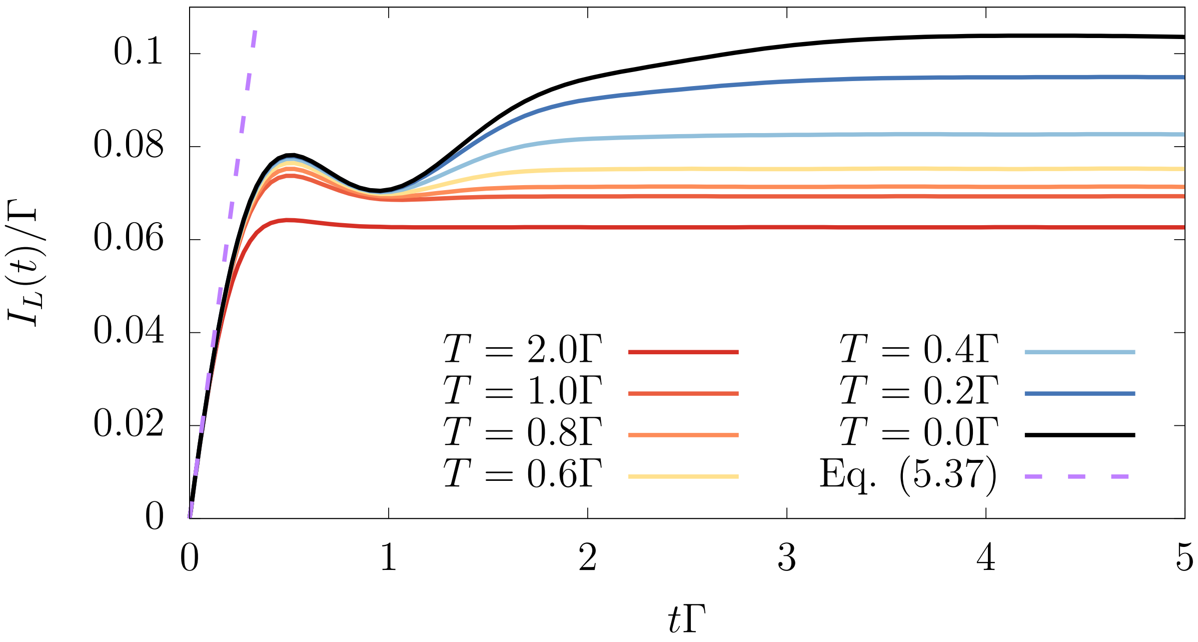
$$\frac{\partial \Pi}{\partial T} = -i\,\Pi * \frac{\partial \Sigma}{\partial T} * \Pi$$





Eckel *et al*, New J. Phys. **12**, 043042 (2010) Werner *et al*, Phys. Rev. B **81**, 035108 (2010)

4.4 Short-time dynamics: T independent !



$\longrightarrow$ short time observables are independent of T:

$$\frac{I(\delta t)}{\Gamma} = (V - U - 2\,\varepsilon)\,\frac{\delta t}{\pi} + (1 - \langle n \rangle_{\rho_0})\left[1 + (U - 2\pi\,\Gamma)\,\frac{\delta t}{\pi}\right]$$

Thank you for your attention !

Summary:

My work has been focused on **open quantum systems** from both a **statistical physics** and a **quantum information** perspective:

- 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)