De-quantizing memory: Non-Markovian dynamics made simple?

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CEA Workshop
The Stochastic Schrödinger Equations
in selected physics problems
December 6, 2011

Overview

1) Physics scope: (our) applications and energy scales

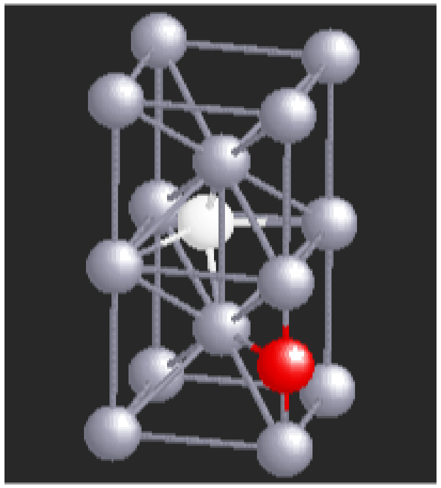
2) Quantum master equations: why go further?

3) Reduced dynamics beyond perturbation theory

4) Some applications

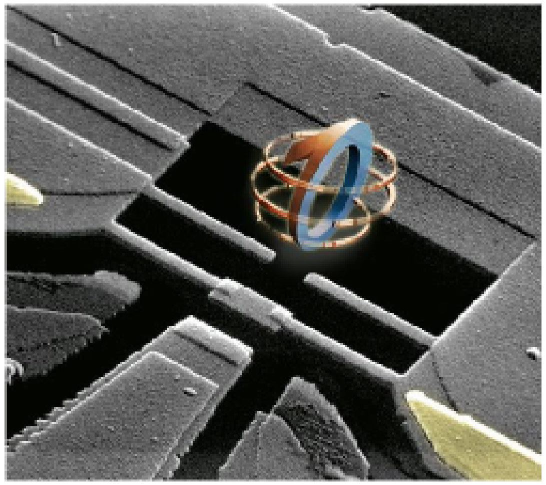
5) Challenges and limitations - stochastic "gears and pulleys"

1. Physics scope: applications and energy scales

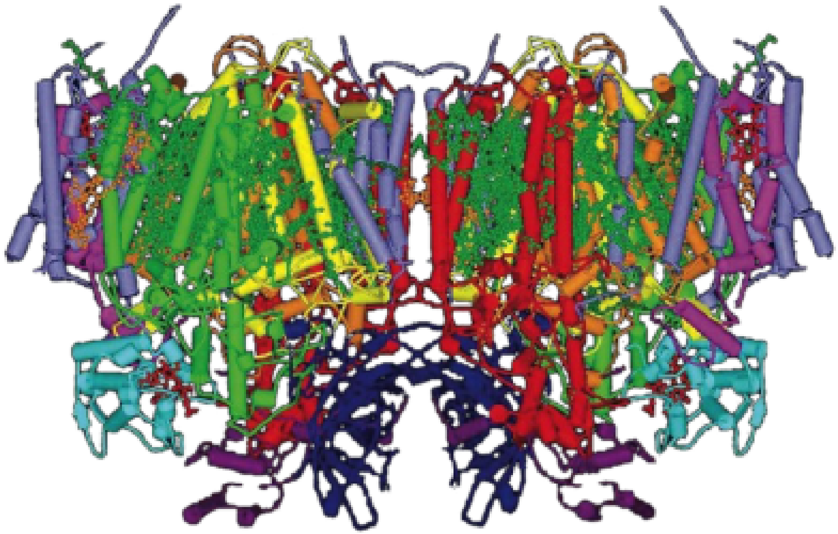


interstitial H

open-system quantum dynamics
in condensed matter



superconducting circuit



photosystem II:
light-harvesting antenna

1. Physics scope: applications and energy scales

• tunneling in solids	~ GHz
• superconducting circuits	~ mK
• biophysics: e.g., photosynthesis	meV to eV
• (photo-)chemical reactions	meV to eV
• mesoscopic transport	zero to eV
• engineering of quantum dynamics	*dynamic*
a.k.a. quantum information processing	

environmental effects: likely non-perturbative, non-Markovian

2. Quantum master equations (telegram style)

Fermis Golden Rule:

$$\Gamma(E) \propto |g_{if}|^2 n(E)$$

- $n(E)$ = density of states
- rate involves temparature

Quantum optical master equation

$$\frac{\partial}{\partial t}\rho = -\frac{i}{\hbar}[H_0, \rho] + \sum_k \left(L_k \rho L_k^\dagger - \frac{1}{2} L_k^\dagger L_k \rho - \frac{1}{2} \rho L_k^\dagger L_k \right)$$

Lindblad operators $L_k \propto \sqrt{\Gamma(E)} \rightarrow$ transitions and dephasing

Stochastic Schrödinger equations

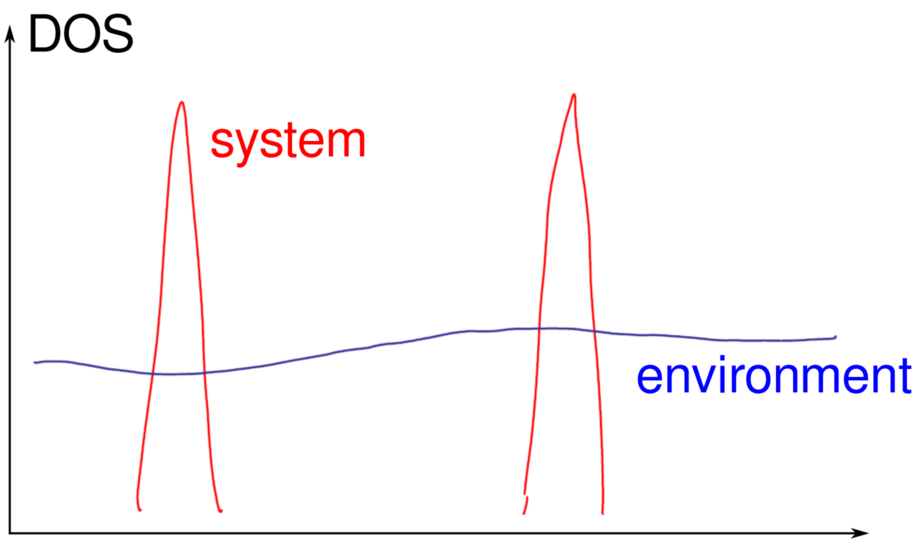
stochastic unraveling of $L_k \rho L_k^\dagger \rightarrow$

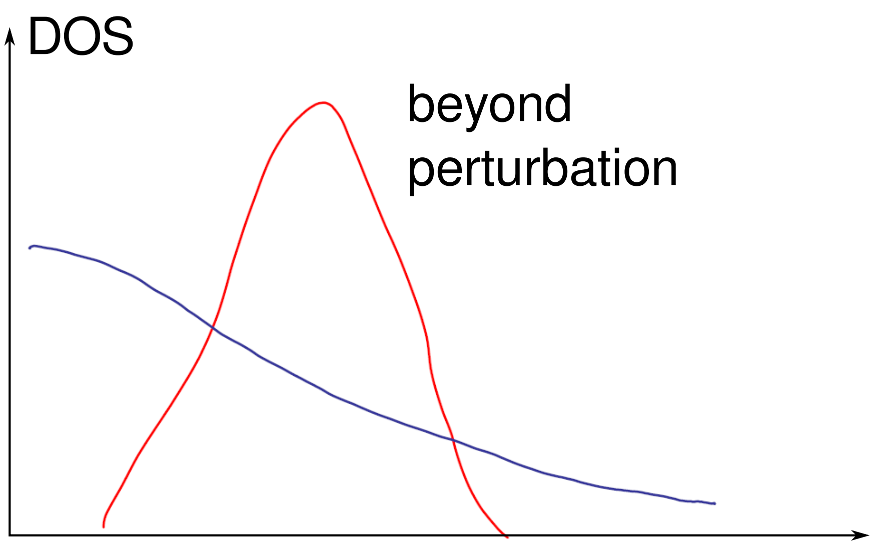
- quantum state diffusion
- quantum jump methods

ρ represented by samples $|\psi\rangle\langle\psi|$

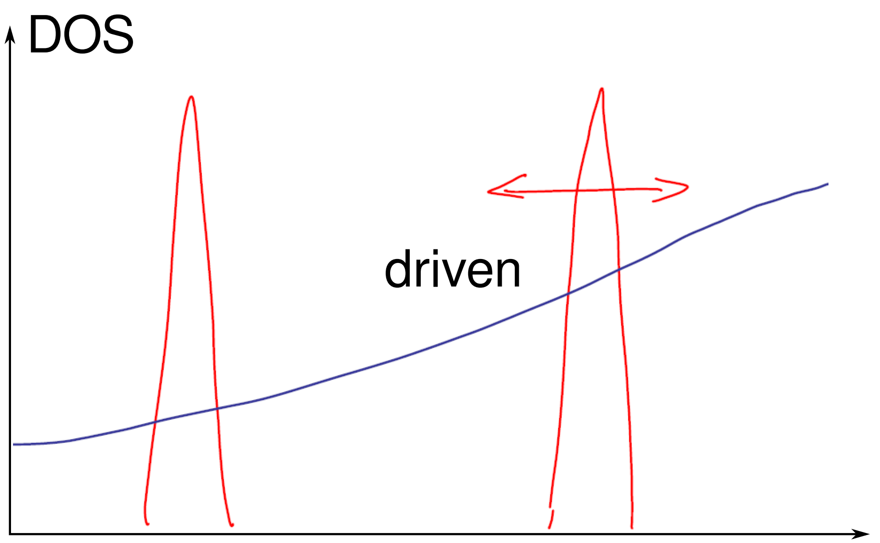
2. Quantum master equations

Condition for Golden Rule: narrow lines vs. flat density of states

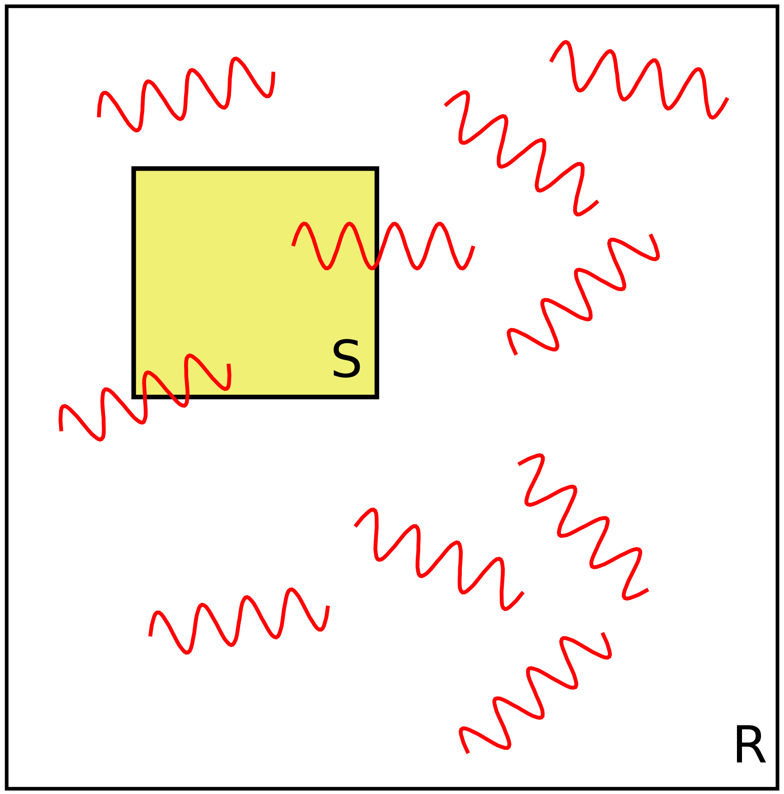




?



3. Reduced dynamics beyond perturbation theory



system-reservoir paradigm

$$H = H_S + H_I + H_R$$

W = density operator in *product* space
$\rho = \mathrm{tr}_R\, W$ = reduced density operator, density in *system* space

propagation:
$\rho(t) = \mathrm{tr}_R\, U(t) W_0 U^\dagger(t) = \mathcal{V}(t)\rho_0$

interaction picture:

$$\mathcal{V}(t)\cdot = \mathop{\mathrm{tr}}_{R} \left\{ \exp_> \left(-\frac{i}{\hbar} \int_0^t dt' H_I(t') \right) (\cdot \otimes W_R) \exp_< \left(+\frac{i}{\hbar} \int_0^t dt' H_I(t') \right) \right\}$$

$\mathcal{V}(t)$ *may* have semigroup properties

3. Reduced dynamics beyond perturbation theory

re-create averages, for separable H_I:

$$H_{\mathrm{I}}(t) = -\hat{q}_{\mathrm{I}}(t)\hat{\xi}_{\mathrm{I}}(t) \quad \rightarrow \quad \tilde{H}(t) = -z(t)\hat{q}_{\mathrm{I}}(t)$$

$z(t)$ = *scalar* noise

Gaussian statistics

"de-quantization" condition:

$$\langle T\hat{\xi}(t)\hat{\xi}(t')\rangle_{\mathrm{R}} \equiv \langle z(t)z(t')\rangle$$

noise is now an exact proxy for the reservoir average:

$$\left\langle \exp_{>}\left(-\frac{i}{\hbar}\int H_{\mathrm{I}}(s)ds\right)\right\rangle_{\mathrm{R}} \equiv \left\langle \exp_{>}\left(-\frac{i}{\hbar}\int \tilde{H}(s)ds\right)\right\rangle$$

... repeat with *pair* of propagators!

3. Reduced dynamics beyond perturbation theory

$\rho_{\text{red}}(t) = \langle \tilde{\rho}(t) \rangle$ — stochastic average over numerical noise

$$\frac{\partial}{\partial t}\tilde{\rho} = -\frac{i}{\hbar}[H_0, \tilde{\rho}] + \frac{i}{\hbar}\xi(t)[q, \tilde{\rho}] + \frac{i}{2}\nu(t)\{q, \tilde{\rho}\}$$

stochastic Liouville-von Neumann equation

noise statistics:

separable:
$\tilde{\rho}(t) = |\psi_1(t)\rangle\langle\psi_2(t)|$

$$\begin{aligned}
\langle \xi(t)\xi(t') \rangle &= \text{Re}\langle \hat{\xi}(t)\hat{\xi}(t') \rangle_{\text{env}} \\
\langle \xi(t)\nu(t') \rangle &= \tfrac{2i}{\hbar}\Theta(t-t')\,\text{Im}\langle \hat{\xi}(t)\hat{\xi}(t') \rangle_{\text{env}} \\
\langle \nu(t)\nu(t') \rangle &\equiv 0
\end{aligned}$$

no system properties

ν is complex with random phase

J.S. and Hermann Grabert 2002

3. Reduced dynamics beyond perturbation theory

Equivalence to influence functionals (Feynman/Vernon 1963):

$$\rho(q_{\rm f},q'_{\rm f};t_{\rm f}) = \int dq_{\rm i}\int dq'_{\rm i}\int_{q_{\rm i}}^{q_{\rm f}}\mathcal{D}[q_1]\int_{q'_{\rm i}}^{q'_{\rm f}}\mathcal{D}[q_2]e^{\frac{i}{\hbar}(S_0[q_1]-S_0[q_2])}$$

$$\times F[(q_1+q_2)/2, q_1-q_2]\ \rho(q_{\rm i},q'_{\rm i};t_{\rm i}) ,$$

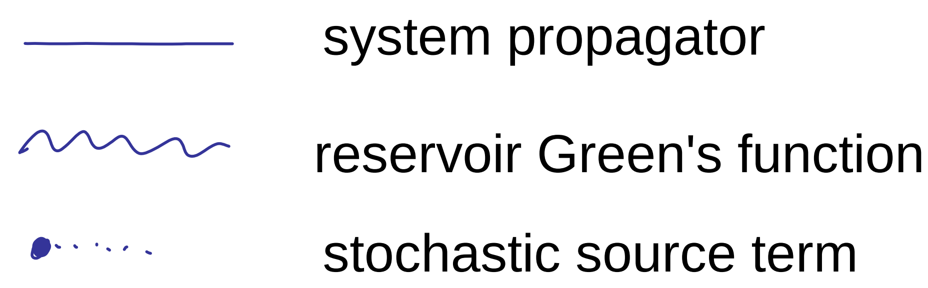
$$F[r,y] = \exp\left(-\hbar^{-2}\int dt\int^{t} dt' y(t)\left[\Re L(t-t')y(t') + i\Im L(t-t')r(t')\right]\right) ,$$

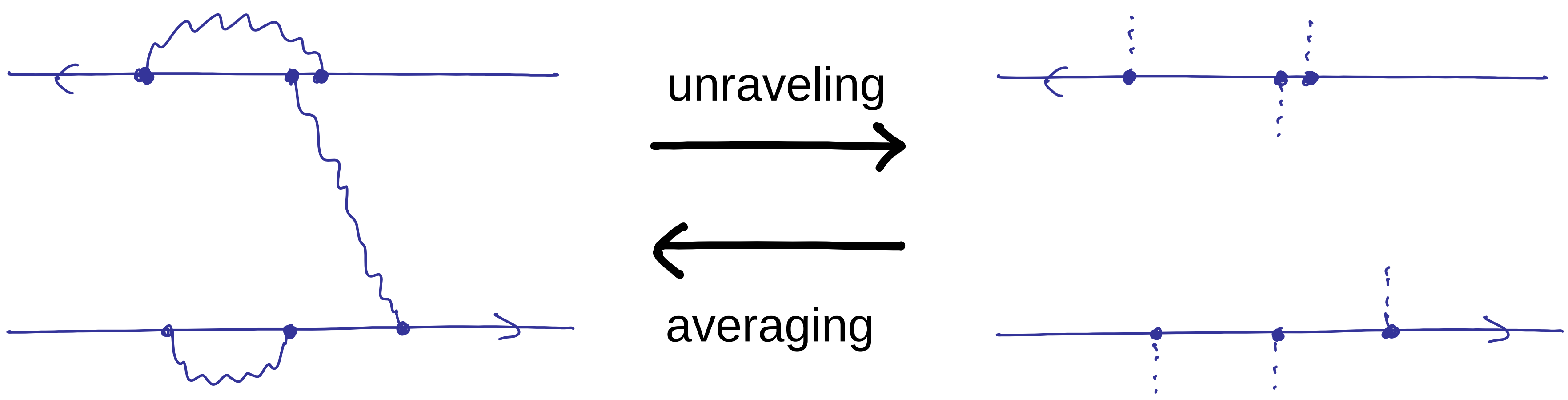
where $L(t-t') = \langle\hat{\xi}(t)\hat{\xi}(t')\rangle_{\rm R}$ is the quantum correlation function of free reservoir fluctuations.

The influence functional *F*[*r,y*] results from the partial trace operation.

It is the *characteristic functional* of the random functions ξ(t) and v(t).

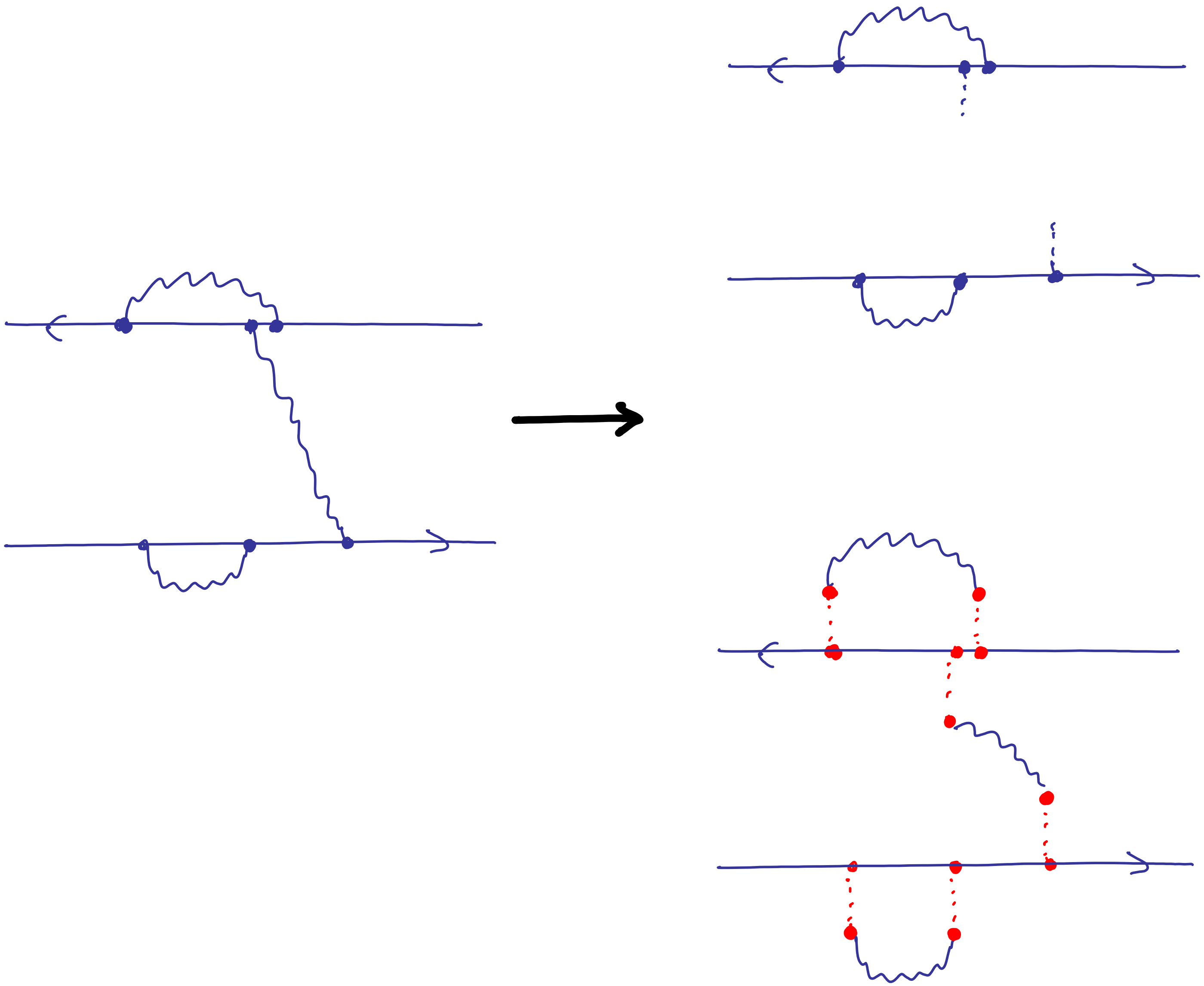
A diagrammatic view





note: influence functional contains *all* higher-order diagrams

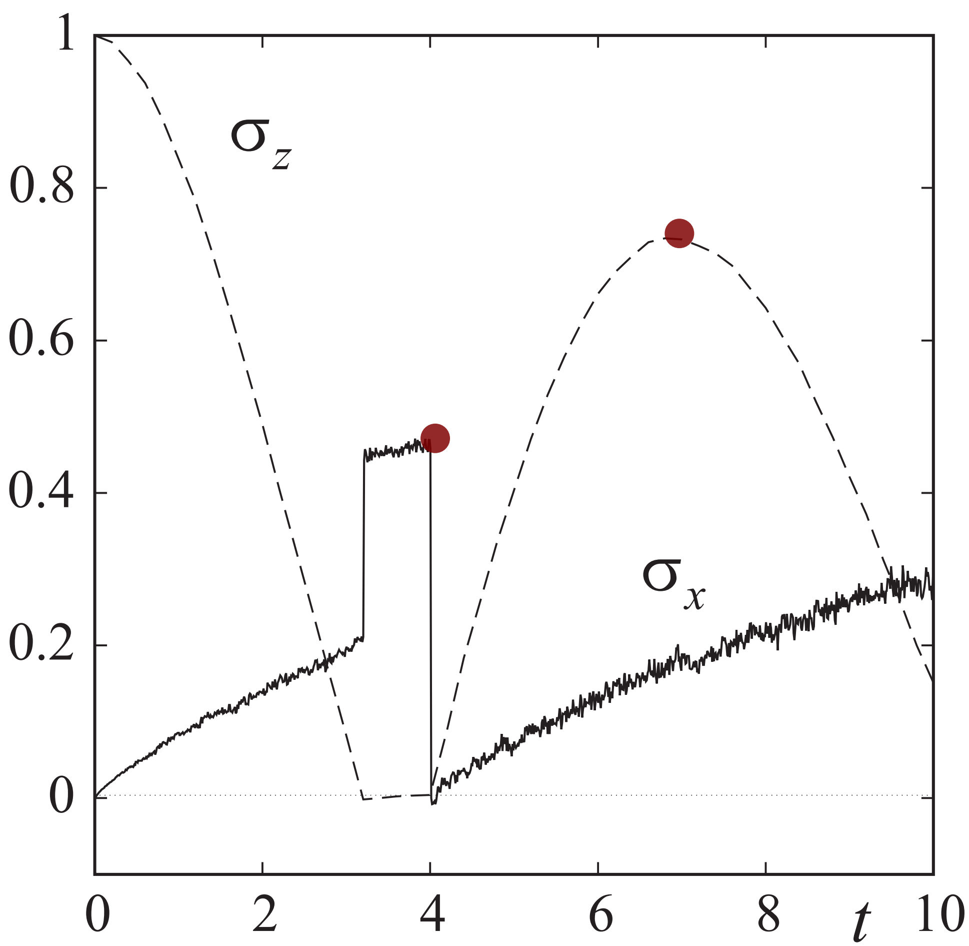
Other unraveling strategies



keep memory
within propagators
(Diosi, Strunz)

"cut apart" vertices
using complex
Wiener processes
(Lacroix, Shao, Zhou)

4. Applications

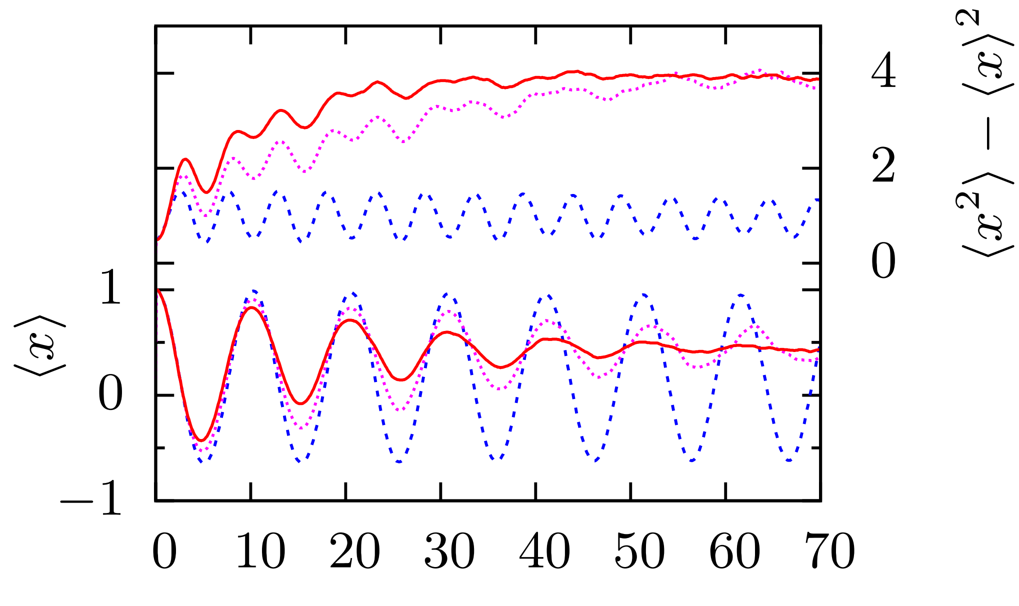


- free precession of a two-level pseudospin in an ohmic environment
- short pulses near t=3 and t=4 interrupt free precession
- higher position of second red dot indicates revival of co-herence: *outward* movement from origin of Bloch sphere

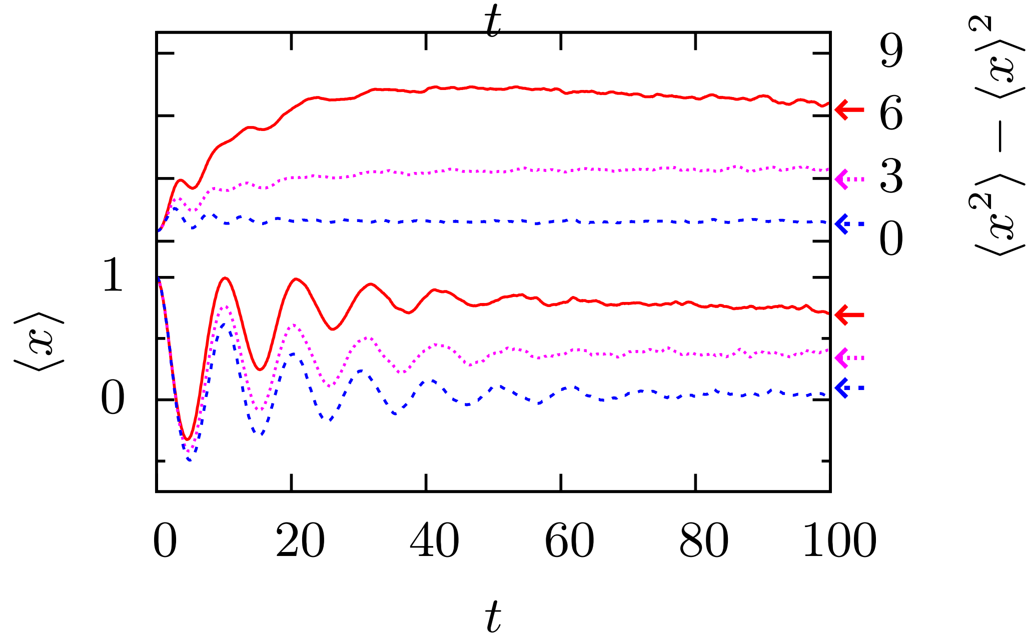
evidence of non-Markovian dynamics

4. Applications

mean and variance of oscillator position for friction η=0 (blue) and for η=0.05 and η=0.1 (magenta and red)



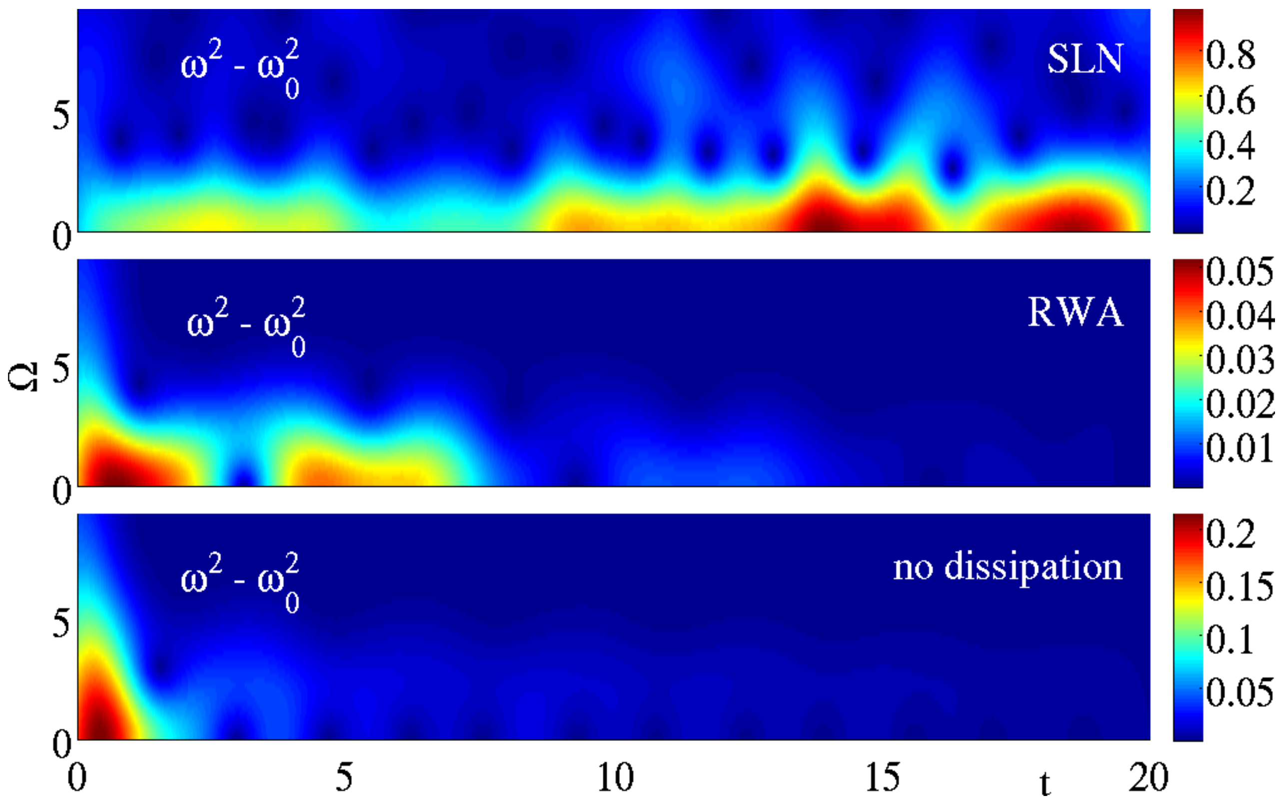
same for varying temperature, kT = 0.1, 1, 2 (blue to red)



semiclassical quantum dissipation (Morse oscillator)

W. Koch, F. Großmann, J.S. and J. Ankerhold, PRL 2008

4. Applications



stoch. Liouville eq.

quantum master eq.

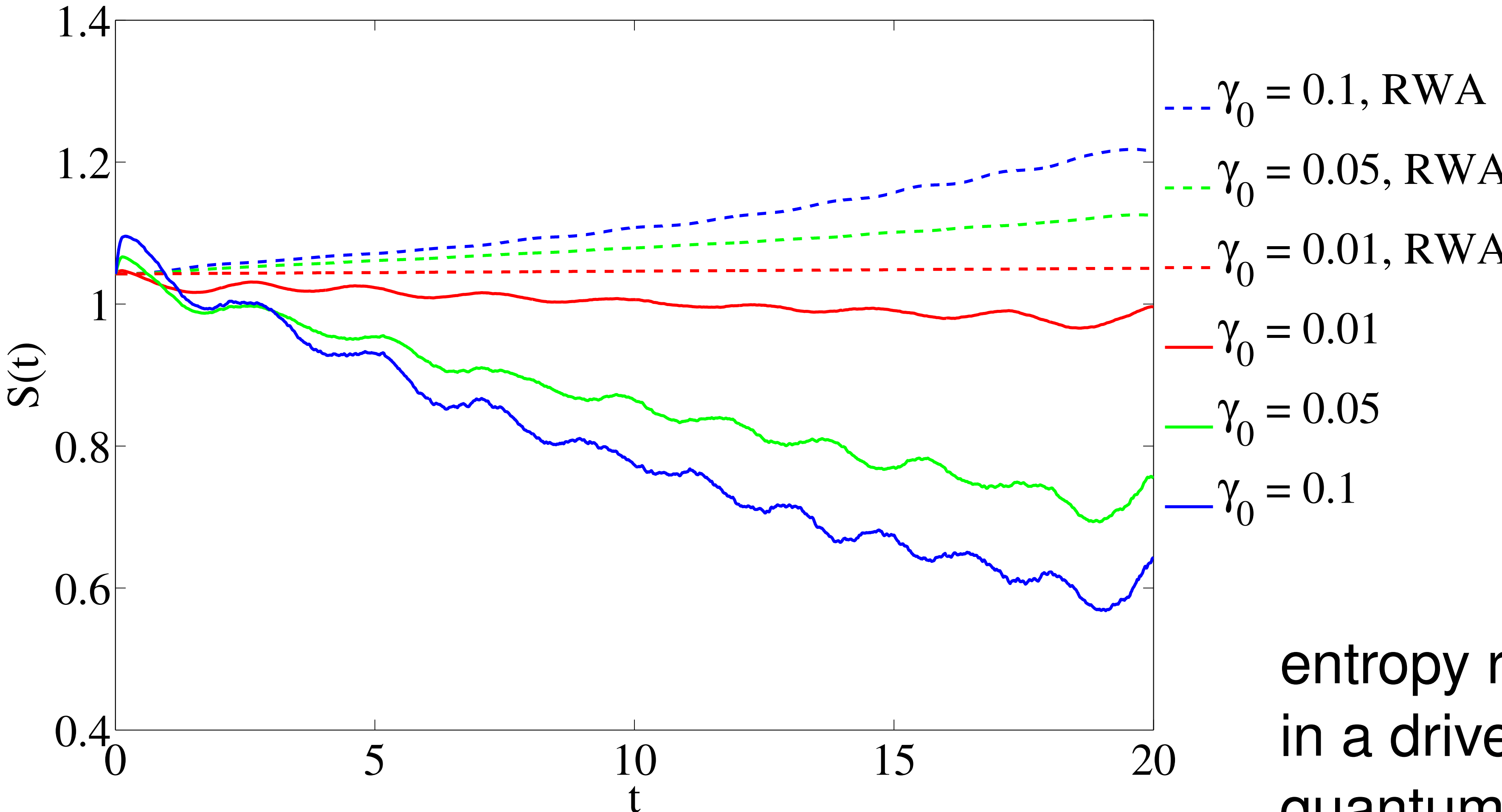
without dissipation

parametric control signal after iteration, windowed Fourier transform

optimal control on a quantum oscillator

R. Schmidt, A. Negretti, J. Ankerhold, T. Calarco, J.S., PRL 2010

4. Applications



entropy reduction in a driven open quantum system

optimal control on a quantum oscillator

R. Schmidt, A. Negretti, J. Ankerhold, T. Calarco, J.S., PRL 2010

5. Challenges and limitations - "gears and pulleys"

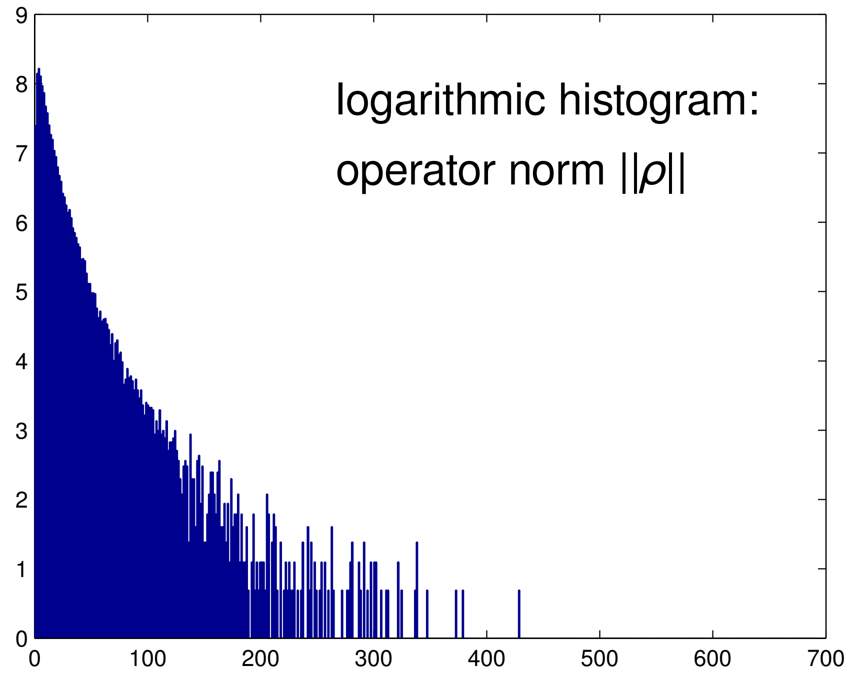
$$\frac{\partial}{\partial t}\tilde{\rho} = -\tfrac{i}{\hbar}[H_0, \tilde{\rho}] + \tfrac{i}{\hbar}\xi(t)[q, \tilde{\rho}] + \tfrac{i}{2}\nu(t)\{q, \tilde{\rho}\}$$

conceptually simple, but *expensive:*

$$\frac{d}{dt}\log \mathrm{tr}\,\tilde{\rho} = i\nu\frac{\mathrm{tr}(\hat{q}\tilde{\rho})}{\mathrm{tr}\,\tilde{\rho}} \approx i q_{\mathrm{char}}\nu$$

-> close similarity to geometric Brownian motion in the complex plane
-> sample trace has exponentially growing variance (!)

geometric Brownian motion:
almost fat-tailed distribution

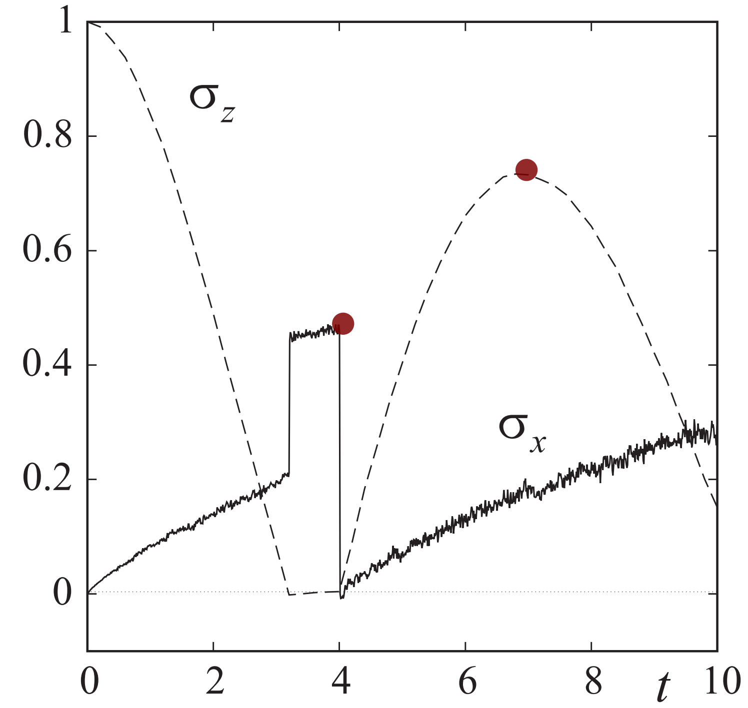


5. Challenges and limitations - "gears and pulleys"

Strategies to keep sample trace "sane":

i) split off a Markovian term from the cross-correlation $\langle \xi(t)v(t') \rangle$.
-> growth rate of sample trace is slow/tolerable on the timescale of the dynamics
-> access to transient dynamics on all relevant timescales, including relaxation and dephasing

used in first example (pseudospin)



5. Challenges and limitations - "gears and pulleys"

Strategies to keep sample trace "sane":

ii) hybrid semi-Markovian method: At low temperature, fluctuations are sluggish, while dynamic response can be fast.

-> Markovian approximation on $\langle \xi(t)v(t') \rangle$ only, keep $\langle \xi(t)\xi(t') \rangle$ as colored noise, now *real-valued*.

-> constant sample trace

$$\frac{d}{dt}\tilde{\rho} = \frac{1}{i\hbar}\Big([H_S, \tilde{\rho}] - \xi(t)[q, \tilde{\rho}]\Big) + \frac{\gamma}{2i\hbar}[q, \{p, \tilde{\rho}\}]$$

~ quantum analogue of Fokker-Planck equation

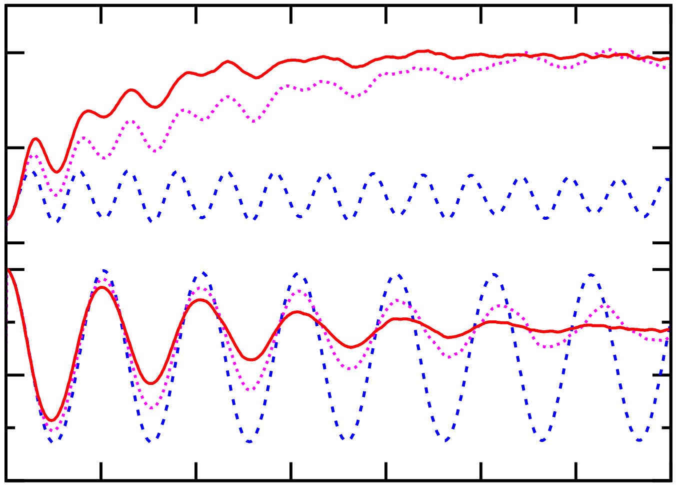
5. Challenges and limitations - "gears and pulleys"

Strategies to keep sample trace "sane":

iii) split off mean-field part from dynamic response.
-> smaller initial growth of sample trace variance
-> potential instability due to nonlinearity

known to be stable near the limits of:
- harmonic systems
- (semi-) classical systems
- weak coupling

applied in second example



5. Challenges and limitations - "gears and pulleys"

Strategies to keep sample trace "sane":

iv) eliminate unneeded correlations of type $\langle$v(t)v(t')$\rangle$.

$$\begin{aligned}
\langle\tilde{\rho}(t)\rangle &= \left\langle \frac{\tilde{\rho}(t)}{\mathrm{tr}\,\tilde{\rho}(t)} \cdot \frac{\mathrm{tr}\,\tilde{\rho}(t)}{\mathrm{tr}\,\tilde{\rho}(t-\tau)} \cdot \frac{\mathrm{tr}\,\tilde{\rho}(t-\tau)}{\mathrm{tr}\,\tilde{\rho}(0)} \right\rangle \\
&\approx \left\langle \frac{\tilde{\rho}(t)}{\mathrm{tr}\,\tilde{\rho}(t)} \cdot \frac{\mathrm{tr}\,\tilde{\rho}(t)}{\mathrm{tr}\,\tilde{\rho}(t-\tau)} \right\rangle \cdot \langle \mathrm{tr}\,\tilde{\rho}(t-\tau)\rangle \\
&= \left\langle \frac{\tilde{\rho}(t)}{\mathrm{tr}\,\tilde{\rho}(t-\tau)} \right\rangle
\end{aligned}$$

constant τ (independent of t)

relative change of $\mathrm{tr}\,\tilde{\rho}$ accumulates increments with *short* correlation time

$$\frac{d}{dt}\log\mathrm{tr}\,\tilde{\rho} = i\nu\frac{\mathrm{tr}(\hat{q}\tilde{\rho})}{\mathrm{tr}\,\tilde{\rho}}$$

"freeze" growth of variance at a timescale τ

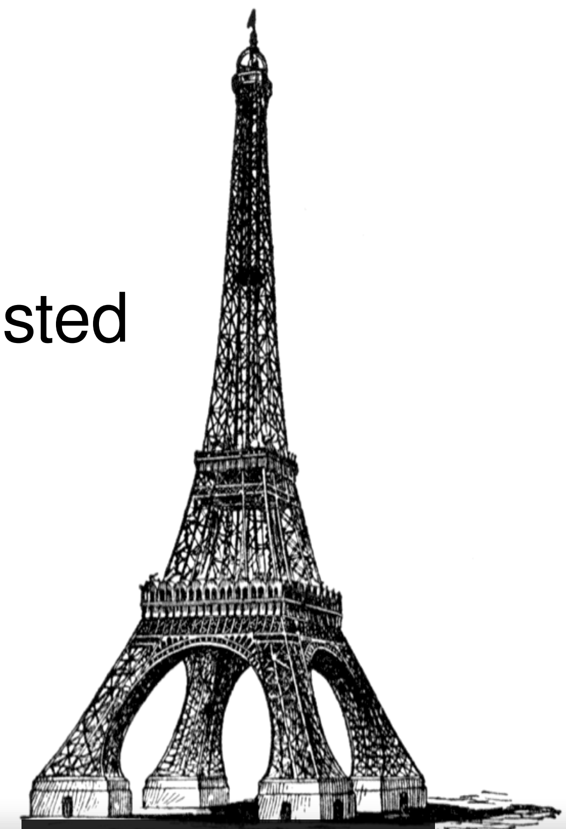
5. Challenges and limitations - "gears and pulleys"

A cartoon conclusion

master equation + SSE

stochastic Liouville equation

time tested



under construction, partly habitable

solid foundation rooted in F.G.R.

broad foundation, based on Gaussian statistics

Outlook:

ad ii): refine semi-Markovian dynamics

ad iv): seek a more efficient way to
eliminate spurious correlations