Work and heat for two-level systems in dissipative environments: Strong driving and non-Markovian dynamics

M. Florencia Carusela

UNGS-CONICET Buenos Aires - Argentina

NESP 2015, ICTS, Bengaluru - India

Collaborators

Rebecca Schmidt
Univ. of Nottingham, UK
Univ. Turku, Finland

Joachim Ankerhold
Ulm University, Germany

Jukka P. Pekola
Aalto University, Finland

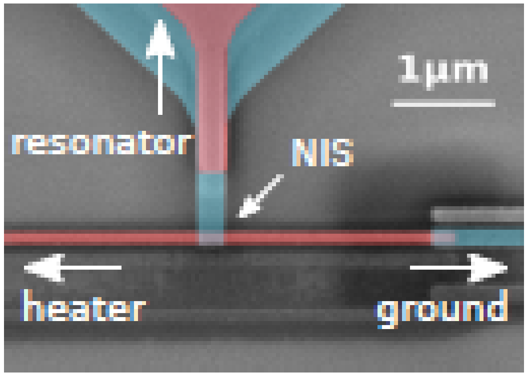
Samu Suomela
Aalto University, Finland

Actual realizations as atomic systems and mesoscopic solid state devices have been put forward to access signatures of quantum thermodynamics

Quantum optical set-ups

Solid-state/Superconducting devices driven strongly by external microwaves

The rf-NIS thermometer



J. P. Pekola et al,
Phys. Rev. Applied (2015)

e.g. current experimental develoments
using ultra-sensitive thermometry (Mhz range)

(To obtain the work monitoring the change in the internal energy and the heat flux)

Importance of non perturbative predictions!!

Theory is challenged to provide tools and methodologies

The problems are related to basically two issues:

- the quantum measurement problem

- the problem of describing dissipative quantum systems at very low temperature, and in presence of also strong external time-dependent fields.

The quantum measurement problem

Two measurement protocol (TMP) provides at least formally a consistent basis for the detection of work and its moments.

Work defined ”operationally” as the difference of eigen-energies before and after an external drive weighted by the thermal initial distribution and driving dependent transition probabilities.

The problem of dissipative quantum systems at very low temperature and in presence of strong external time-dependent fields.

Perturbative approaches

Lindblad type of master equation (LME)

Quantum Jump approach (QJ)

Weak S-B coupling . Markov approximation

Driving has NO impact on the dissipator (weak driving)

Neglect fast oscillations (RWA / Sec.App.)

Quantum Jump Method

The dynamics $\left|\Psi(t)\right\rangle \rightarrow \left|\Psi(t+\Delta t)\right\rangle$ is constructed according to sequences of jumps between energy levels with transition probabilities by the corresponding Hamiltonian (Monte Carlo procedure)

Change in system energy is monitored by recording the last photon exchange before and after the drive (Two times projective measurements). And heat flow from photon exchange during the drive.

[Mølmer, Castin & Dalibard, JOSA B (1993);
Badescu, Ying & TA-N, PRL (2001);
Hekking & Pekola, PRL (2013)]

Lindblad master equation

$$\dot{\rho} = -\frac{i}{\hbar}[H_S(t), \rho] + \sum_{k=0}^{1} \left(L_k \rho L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho\} \right)$$

Lindblad operators and transition rates

(for TLS)

$$L_0 = \sqrt{\gamma_{0,1}}\,|0\rangle\langle 1|$$

$$L_1 = \sqrt{\gamma_{1,0}}\,|1\rangle\langle 0|$$

$$\gamma_{0,1} = \frac{\eta}{2}\Delta\left[1 + \coth\left(\Delta\hbar\beta/2\right)\right],\ \gamma_{1,0} = \gamma_{0,1}e^{-\Delta\hbar\beta}$$

Exact numerical formulation →

Stochastic Liouville-von Neumann equation (SLN)

Stochastic Liouville-von Neumann equation

$$\dot{\rho}_Z = -\frac{i}{\hbar}\left[H_S, \rho_Z\right] + \frac{i}{\hbar}\xi(t)\left[q, \rho_Z\right] + \frac{i}{2}\nu(t)\left\{q, \rho_Z\right\}$$

- Correlation functions of complex noise forces ξ(t) and ν(t) reproduced the complex-valued and non-local in time force autocorrelation of the bath.

  $\langle \xi(t), \xi(t') \rangle$ matches the quantum noise of R

  $\langle \xi(t), \nu(t') \rangle$ matches the dynamical response of the environment

  $\langle \nu(t), \nu(t') \rangle$ vanish

- Holds for a single noise realization $\boldsymbol{Z} \equiv \{\xi, \upsilon\}$
- Physical reduced density ρ(t) is gained by averaging over large number of noise realizations $\rho(t) = \mathbf{E}\left[\rho_Z\,(\mathbf{t})\right]$
- Full non-Markovian dynamics captured in ρ(t)
- General external drivings easily taken into account.

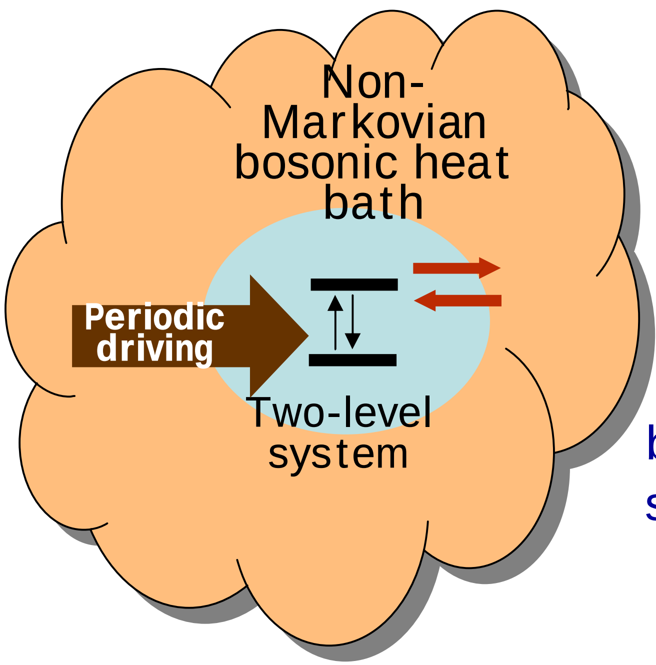
Jürgen T. Stockburger et. al, PRL 88, (2002)
R. Schmidt et al, PRL 09 (2011)

Schemes to obtain work
(two different "experimental" situations)

LME, SNL → dynamics of the power operator

QJ → monitors the energy exchange with the reservoir (photon emission/absortion)

TLS inmersed in a bosonic bath (spin-boson model)



$$H(t) = H_S + H_I + H_R$$

$$-\hbar\frac{\Delta}{2}\sigma_x + \lambda_0 \sin(\Omega t)\sigma_z$$

bare + control system

System-bath interaction $\propto \sigma_z$

Reservoir described by inversed thermal energy β and spectral density

$$J(\omega)=\eta\omega \Big/ \left(1+\omega^2/\omega_c^2\right)^2$$

Moments of Work

Work distribution
(according TMP)

$$p(W) = \sum_{E_i, E_f} \delta[W - (E_f - E_i)] P[E_f, E_i]$$

Power Operator

$$P_W = \frac{\partial H_S}{\partial t} = \frac{\partial H_S}{\partial \lambda} \dot{\lambda}(t)$$

$$\left\langle W \right\rangle_t = \int_0^t ds \left\langle P_W^H(s) \right\rangle$$

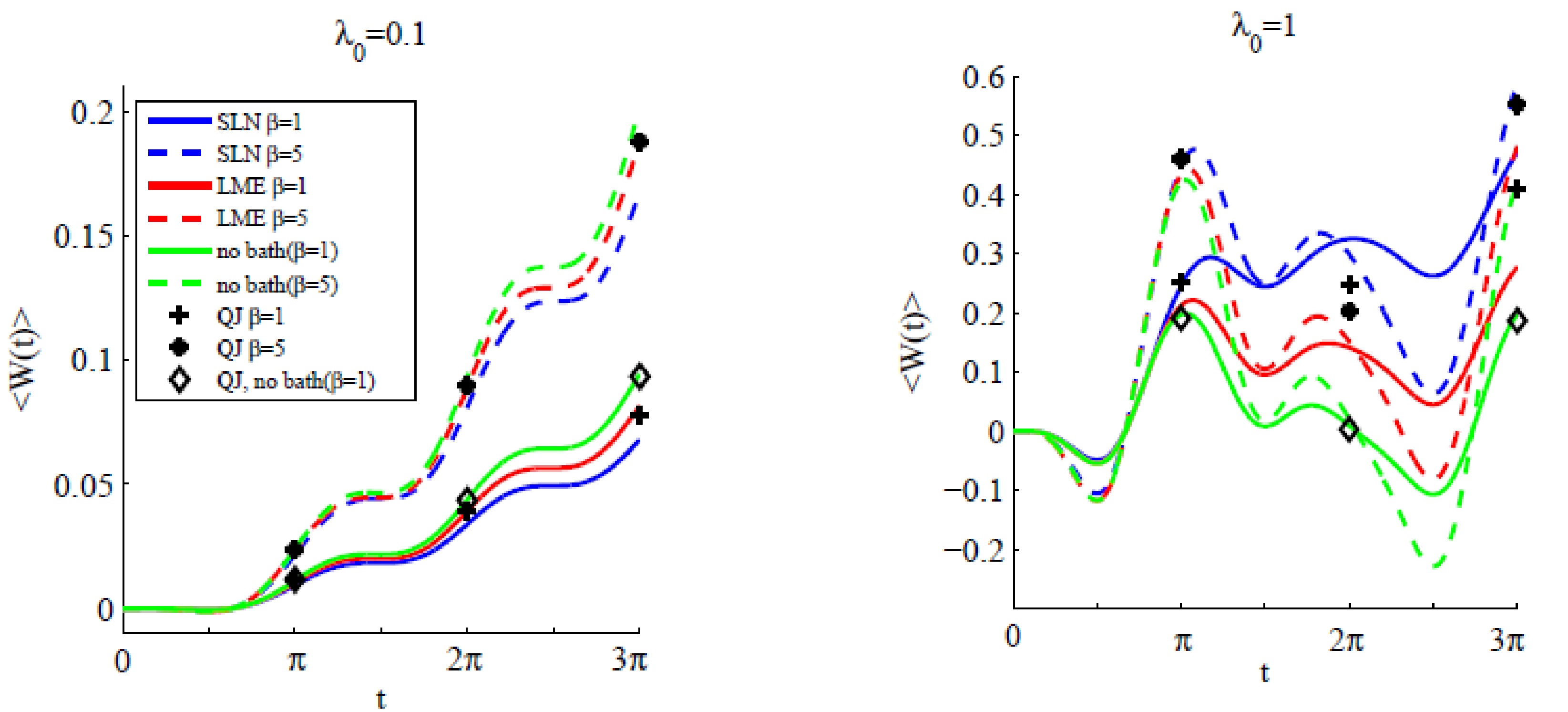
$$\left\langle W^2 \right\rangle_t = 2\int_0^t ds \int_0^s du \, \mathrm{Re}\left\{ \left\langle P_W^H(s) P_W^H(u) \right\rangle \right\}$$

Suomela et. al, PRB 90 (2014)

First Moment

$$\langle W(t)\rangle = \int_0^t ds\,\dot{\lambda}(s)\langle\sigma_z(s)\rangle$$

Stronger driving



Analytic results

Weak driving and at or close to resonance $\Delta=\Omega$

$$H'_S(t) \approx H'_{RWA}(t) = \frac{\hbar\Delta}{2}\sigma_z + i\frac{\lambda_0}{2}\left(e^{-i\Omega t}\sigma_+ + e^{i\Omega t}\sigma_-\right)$$

$$\frac{\langle W\rangle_N}{\hbar\Omega} \approx (2P_g-1)\sin^2\left(\frac{N\pi\bar{\lambda}_0}{2}\right)\left(1-\frac{\bar{\lambda}_0^2}{4-\bar{\lambda}_0^2}\right)$$

Strong driving → Perturbative treatment of rotated TLS ($\lambda_0 >> \hbar\Delta$)

$$H'_S(t) = \frac{\hbar\Delta}{2}\sigma_x - \lambda_0\sin(\Omega t)\sigma_z$$

Fast sweep through Landau-Zener region (velocity $\lambda_0\,\Omega$)

$$\frac{\langle W\rangle_N}{\hbar\Omega} = (2P_g-1)\frac{\bar{\lambda}_0 J_0(\bar{\lambda}_0)}{1-J_0(\bar{\lambda}_0)^2}\cos(2\pi N)\sin[2\pi N J_0(\bar{\lambda}_0)]$$

In the limit of

very strong driving

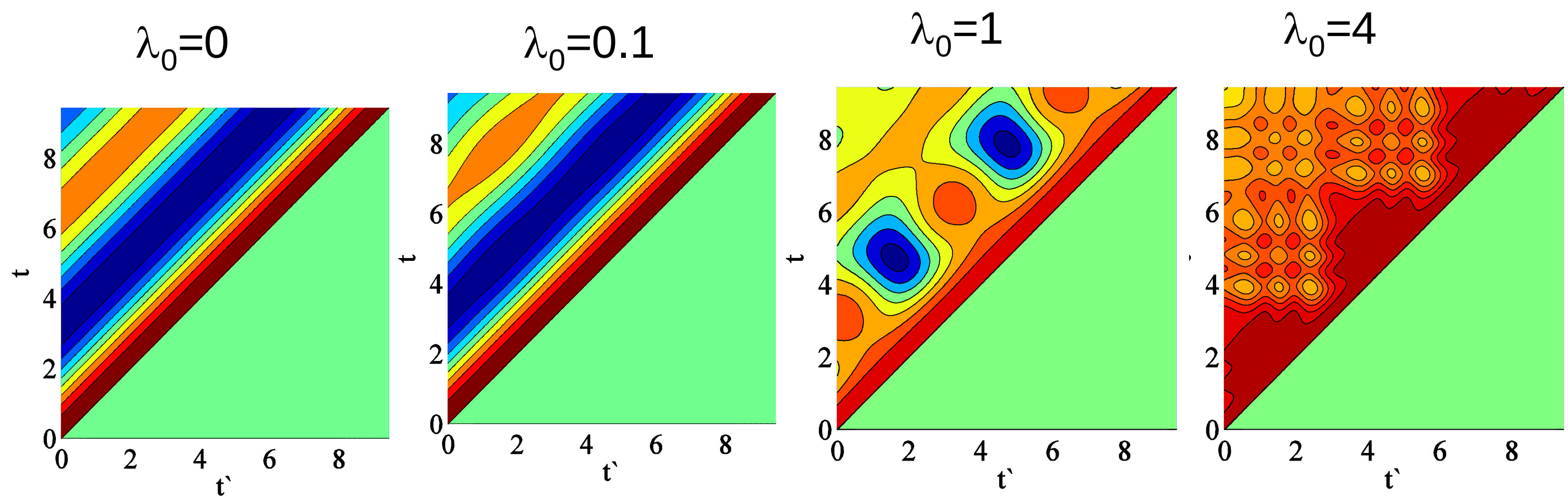
$$\left.\frac{|\langle W\rangle_N|}{\hbar\Omega}\right|_{\bar{\lambda}_0\gg 1} \leq (2P_g-1)4N$$

Energy saturation of TLS !

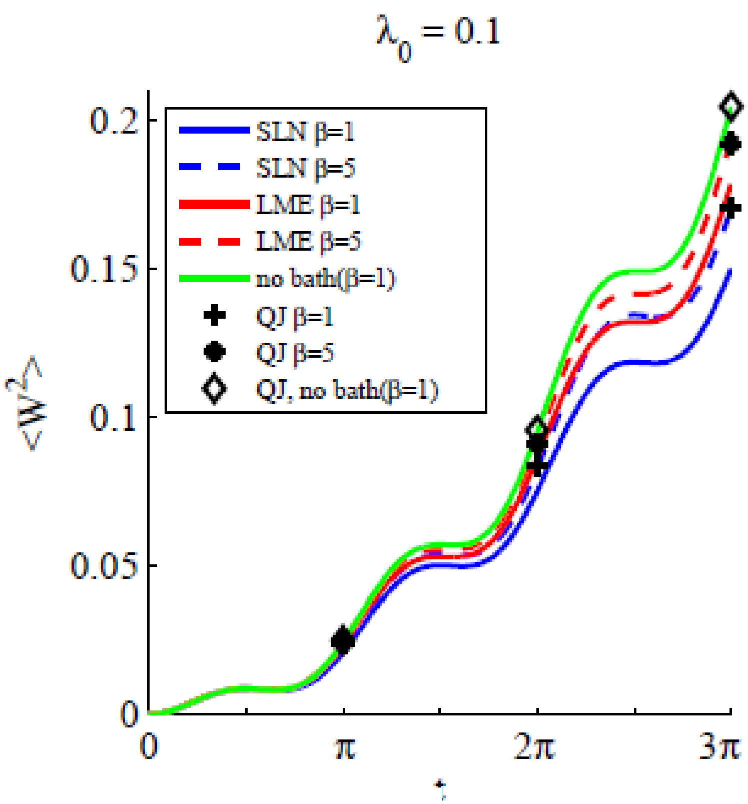
Second Moment of work

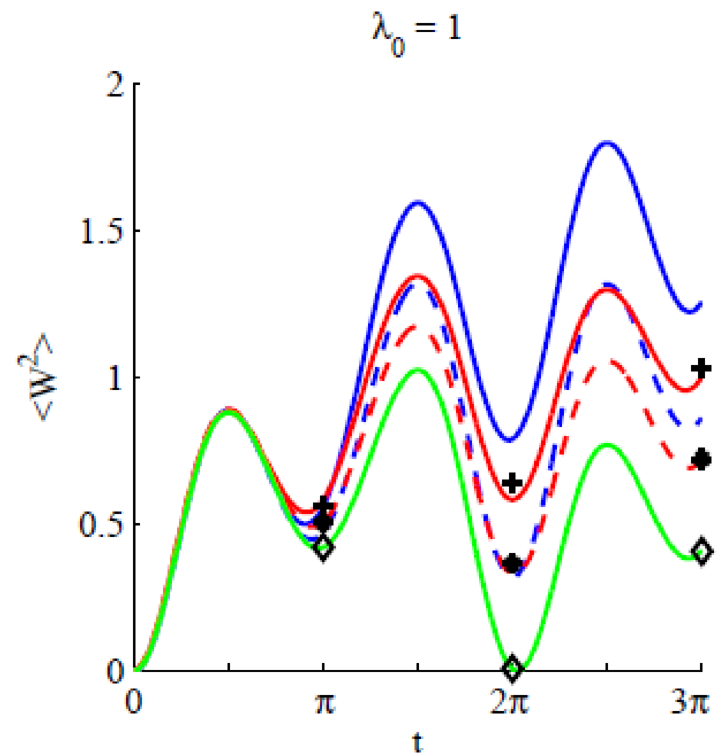
$$\langle W^2(t)\rangle = 2\int_0^t ds \int_0^s du\ \dot{\lambda}(s)\dot{\lambda}(u)\mathrm{Re}\left\{\langle\sigma_z(s)\sigma_z(u)\rangle\right\}$$

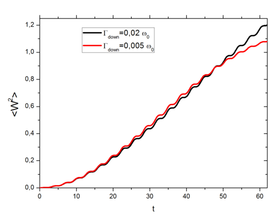
Time ordered two-time correlator



Stronger driving







R.Schmidt, **MFC** , J.P.Pekola,S.Suomela,J.Ankerhold Phys. Rev. B 91, (2015)

Analytic results

Weak driving

$$\frac{\langle W^2\rangle_N}{(\hbar\Omega)^2} = \sin^2(N\pi\bar{\lambda}_0/2)$$

Indep. of initial population *Pg*

Limited by level splitting

Strong driving

$$\frac{\langle W^2\rangle_N}{(\hbar\Omega)^2} = 2\bar{\lambda}_0^2\,\frac{J_0(\bar{\lambda}_0)^2}{[1-J_0(\bar{\lambda}_0)^2]^2}\;\{1-(-1)^N\cos[N\pi J_0(\bar{\lambda}_0)]\}$$

$$\left.\frac{\langle W^2\rangle_N}{(\hbar\Omega)^2}\right|_{\bar{\lambda}_0\gg 1} \approx \begin{cases} N^2\cos^4(\bar{\lambda}_0-\frac{\pi}{4}) & , \; N \text{ even} \\ \frac{8\bar{\lambda}_0}{\pi}\cos^2(\bar{\lambda}_0-\frac{\pi}{4}) & , \; N \text{ odd} \end{cases}$$

→ with total driving time.

→ with λ_0

R.Schmidt, **MFC**, J.P.Pekola, J.Ankerhold,(2015)

Heat Flux

$$\langle W \rangle_t = \int_0^t du \left\langle \frac{\partial H_D^H(u)}{\partial u} \right\rangle$$
$$= \Delta E(t) + \frac{i}{\hbar} \int_0^t du \left\langle \left[H_0^H(u), H_I^H(u) \right] \right\rangle$$

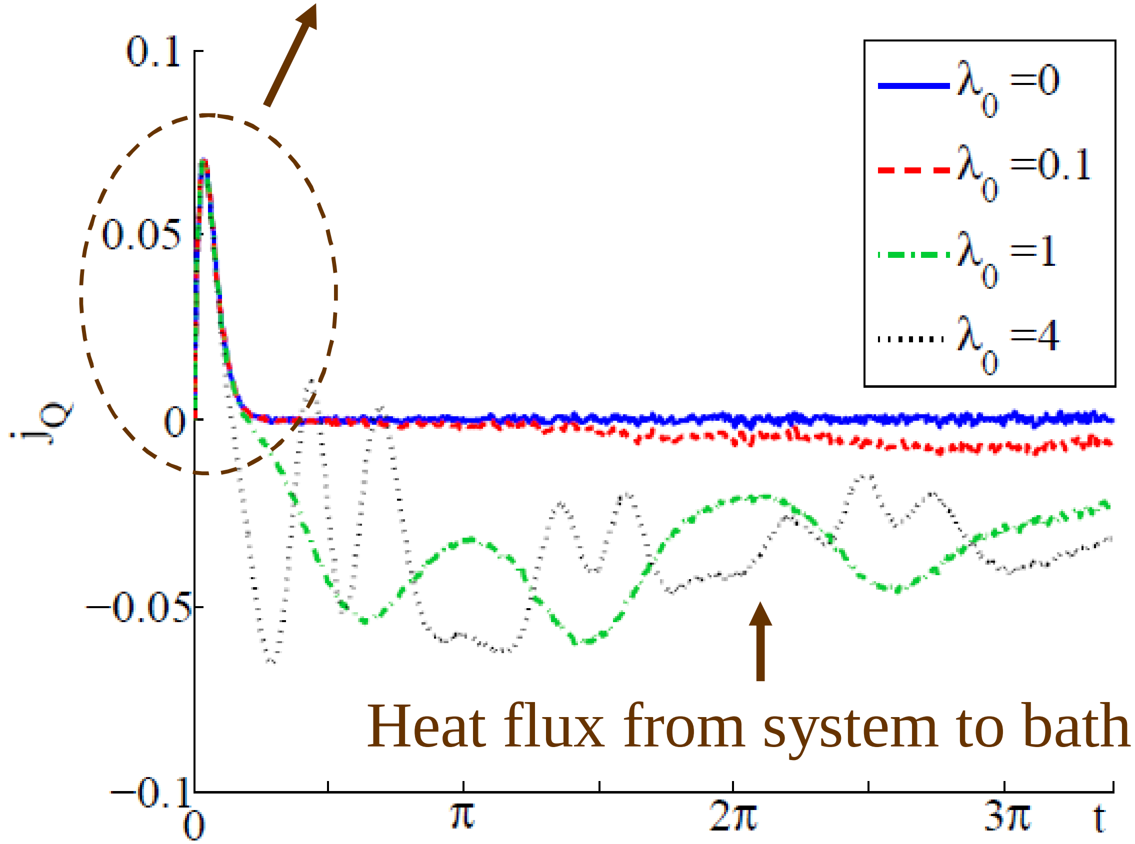
$$\langle Q(t) \rangle = \int_0^t ds \ j_Q(s)$$

Heat

In **SLN** framework: $$j_Q(t) = -\Delta \, \boldsymbol{E}\left[\xi(t) \langle \sigma_z(t) \rangle \right]$$

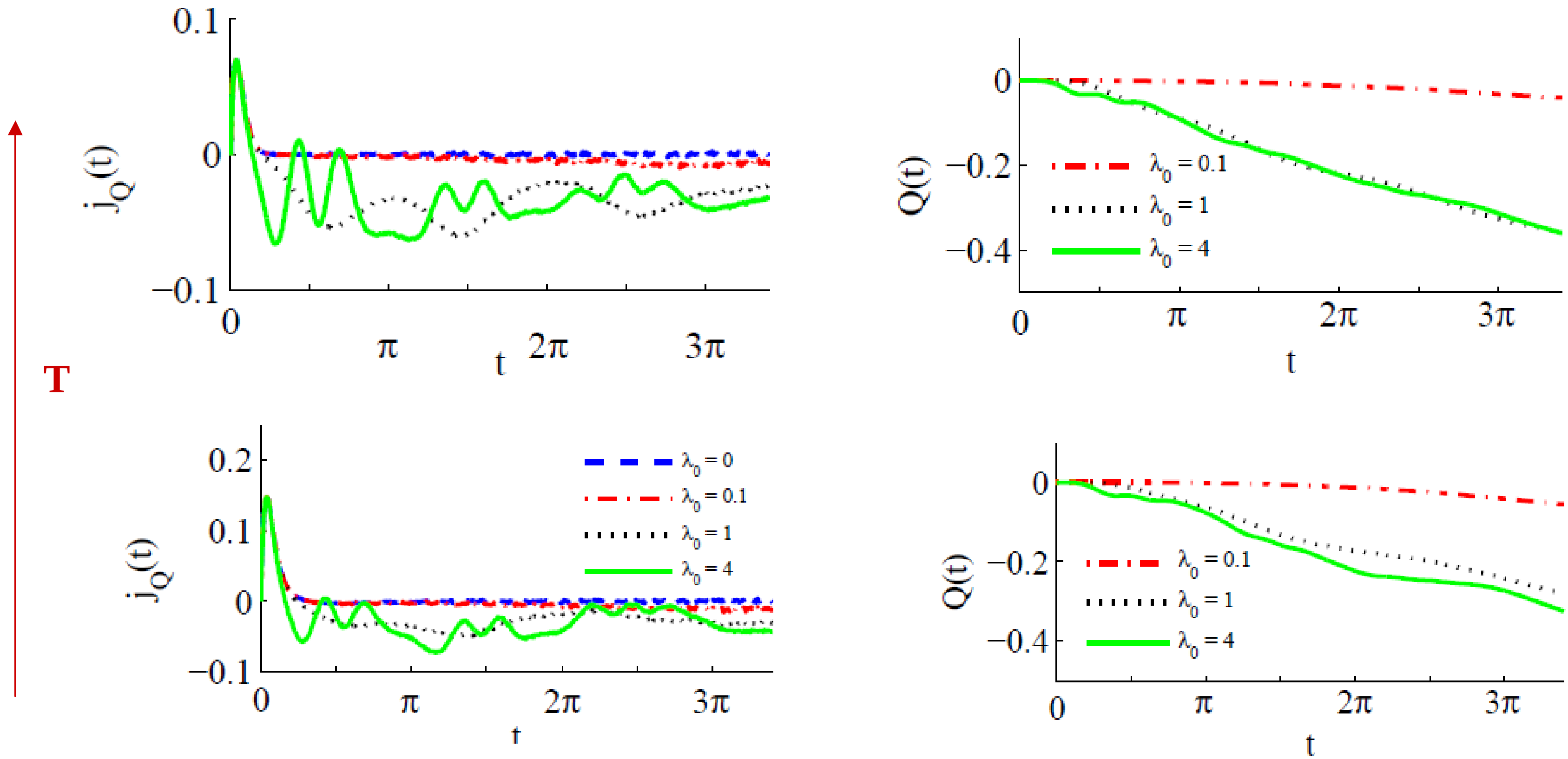
In **LME** framework: $$j_Q(t) = Tr\left[L(\rho(t)) H(t) \right]$$

Initial heat flux from bath to system due to factorizing initial condition (SNL) to establish proper system-bath correlations



Heat flux from system to bath

R.Schmidt, **MFC**, J.P.Pekola, S.Suomela, J.Ankerhold (2015)



According to $Q = \langle W \rangle - \Delta E$ the exchanged heat is limited by the maximal change in internal energy $|\Delta E| \le \hbar\Delta_0$ and the maximun work

For λ_0>>1 $|Q|/\hbar\Omega \le (2P_g - 1)4N$

→ independent of the driving amplitude

Upper bound for the heat exchanged !!

Factorizing initial state

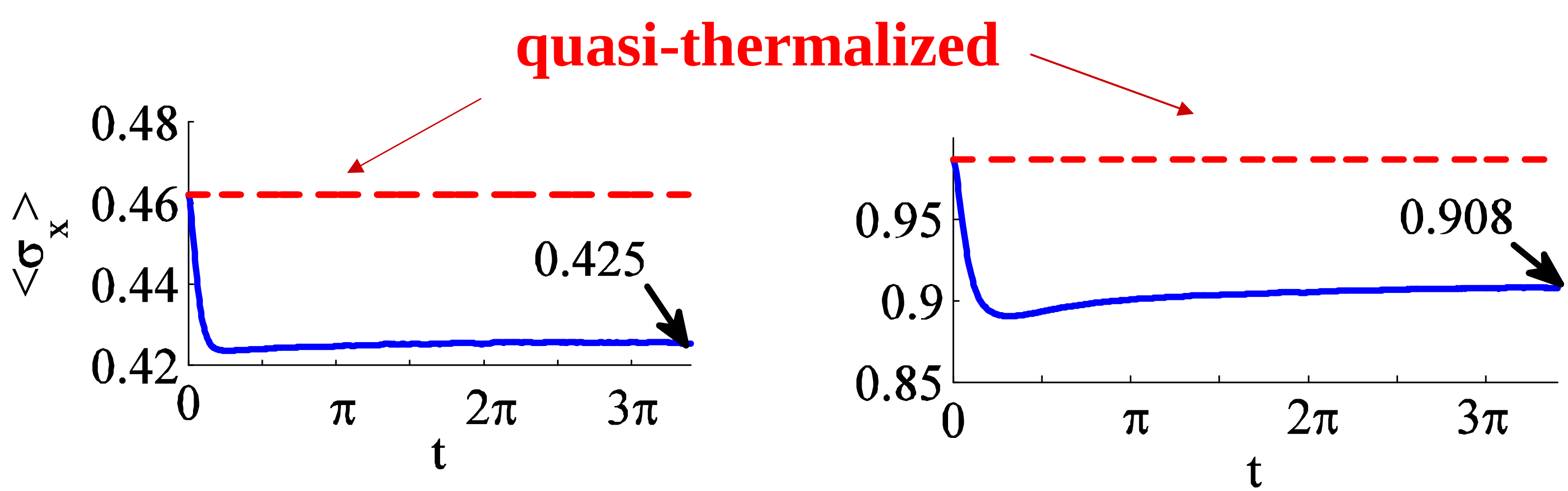
$$W(0) = \rho(0) \otimes \frac{e^{-\beta H_R}}{Z_R}$$

$$\rho(0) = \frac{e^{-\beta H(0)}}{Z_0}$$

**In actual experiment,
the state of the compound
is a correlated thermal eq.**

$$\rho_\beta = Tr\left\{ e^{-\beta H(0)} \big/ Z \right\}$$

Thermalization of $\langle\sigma_x\rangle$ according to the SLN starting from an initially factorizing state with ρ(0) in absence of external driving → full equilibration process



Several questions…

- How reliable are the approximate methods to predict W from Q and ΔE ?

- j_Q due to initial correlations is of the order of j_Q due to driving..

Factorized initial condition may spoil theoretical predictions

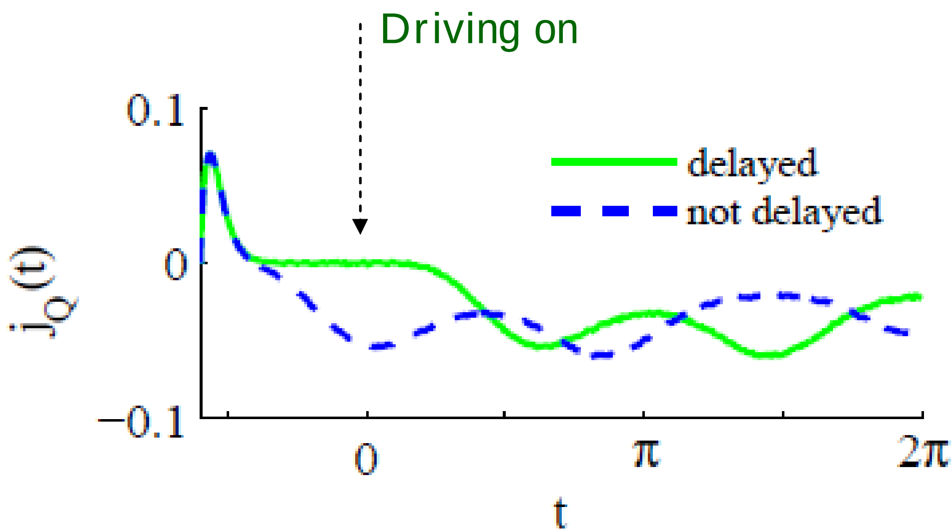
- Is it possible to separate time scales on which correlations are established from those on which driving related phenomena occur?

Yes…at least for weak to moderate driving this separation exists:

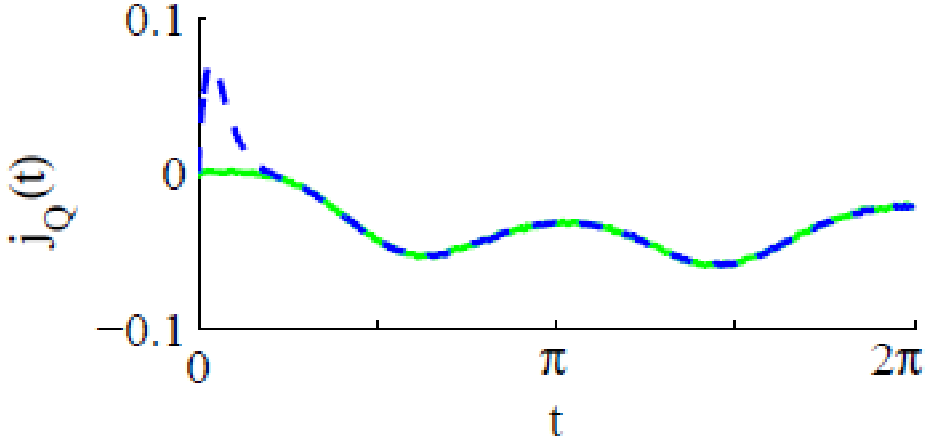
$$\mathbf{Q = Qcorr + Qdriv}$$

Heat due to missing IC

Heat due to driving

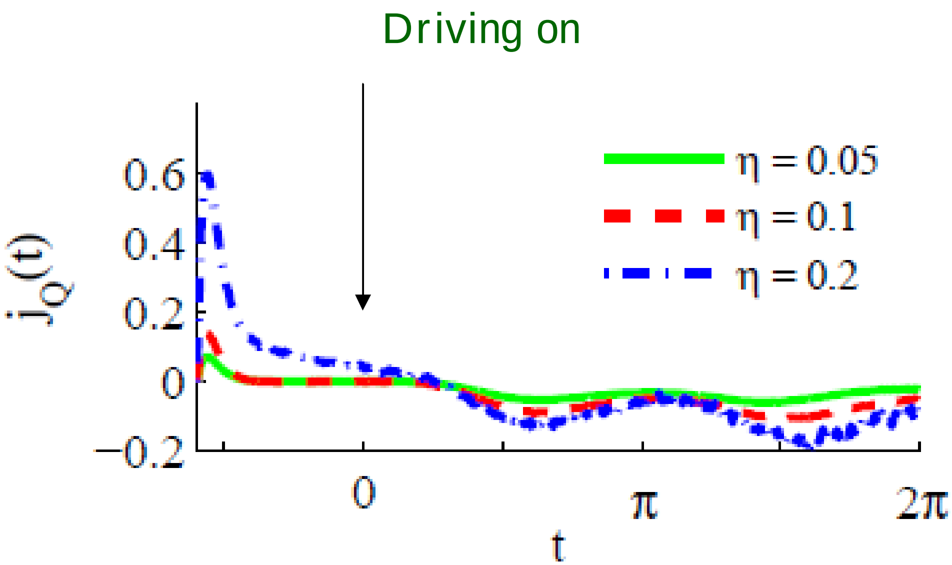


factorized initial state (FIS)



Factor. initial state

Correlated initial state (CIS)



Relevant time scales overlap → Non-perturbative methods, as SNL mandatory !

Evolves S with NO driving, from a FIS → Equilibration sets in → CIS → Dynamics in presence of driving is monitored

Summary

- TLS far from thermal equilibrium in the context of work and heat production.
- Exact treatment required when non-Markovian dynamics and driving are strongly correlated.
- We exploited the equivalence of the TMP and the formulation of W and W^2 in terms of the power operator with properly defined initial states.
- Strong dependence of the heat exchanged on initial state, al least on a transient timescales

Thank you

and

Thanks to organizers !