Numerical path-integral methods for open quantum systems

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NQSTI
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Overview

Part II: Numerical path-integral methods for open quantum systems

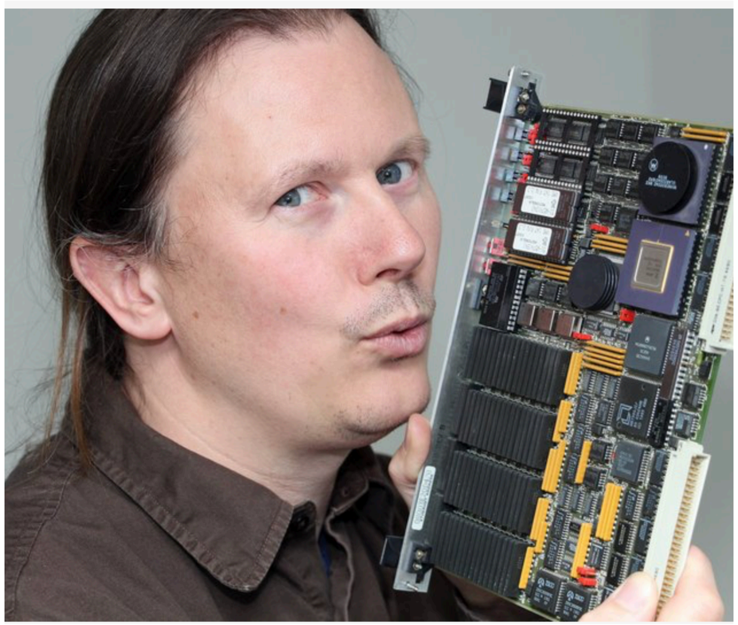
1. Quasiadiabatic propagator path integral QUAPI

   general idea and method

2. Iterative summation of paths: numerically exact results
3. QUAPI as a tensor network: TEMPO
4. Recent examples & applications:
   - dissipative quantum XOR gate
   - superconducting qubit coupled to a SQUID as readout device
   - sub-Ohmic bath and quantum-1/f noise in superconducting qubits
   - superconducting qubits exposed to non-commuting baths

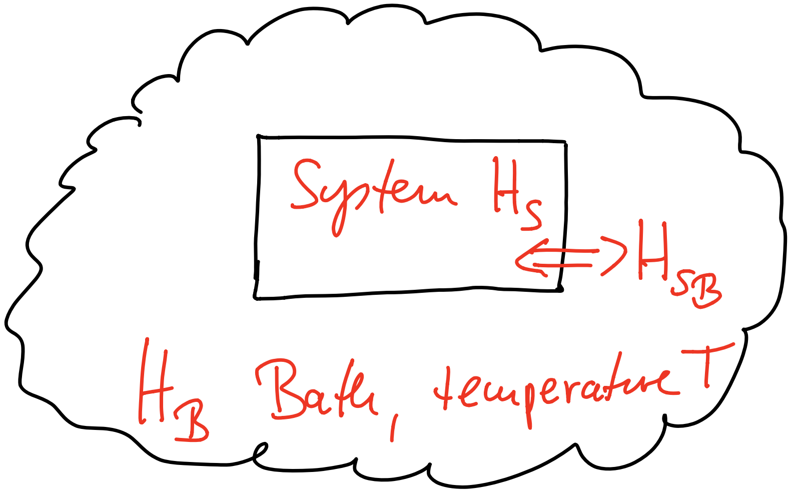
Acknowledgements

Dr. Florian Otterpohl



Prof. Peter Nalbach

System-bath model



$$H_{\text{tot}} = H_S(t) + H_B + H_{SB}$$

System: (for example)

$$\mathbf{H}_{\text{S}}(t) = \frac{\mathbf{p}^2}{2\mathcal{M}} + V(\mathbf{q}, t)$$

Bath + interaction:

$$\mathbf{H}_{\text{B}} = \sum_{j=1}^{\mathcal{N}} \mathbf{H}_j(\mathbf{q}) = \sum_{j=1}^{\mathcal{N}} \frac{1}{2} \left[\frac{\mathbf{p}_j^2}{m_j} + m_j \omega_j^2 \left(\mathbf{x}_j - \frac{c_j}{m_j \omega_j^2} \mathbf{q} \right)^2 \right]$$

- set of uncoupled harmonic oscillators
- bilinear coupling to the system
- effect of bath can be strong since (infinitely) many oscillators couple to system
- counter term: repair for potential renormalization due to bath coupling

Initial condition for system-plus-bath:

$$\mathbf{W}(t_0) = \rho_{\text{S}}(t_0) \otimes \rho_{\text{B}}^0$$

- required for dynamics
- uncoupled at t=0
- instantaneous switching on at t=0+

$$\rho_{\text{B}}^0 = Z_{\text{B}}^{-1} \exp\left(-\beta \mathbf{H}_{\text{B}}^0\right)$$

Bath spectral density

All bath parameters come in a specific combination: bath spectral density:

$$J(\omega) = \frac{\pi}{2} \sum_{j=1}^{\mathcal{N}} \frac{c_j^2}{m_j \omega_j} \delta(\omega - \omega_j)$$

due to non-commuting position & momentum

Continuum limit: $\langle \mathbf{\Gamma}(t) \mathbf{\Gamma}(0) \rangle_{\mathrm{B}} = \hbar L(t) = \frac{1}{\pi} \int_0^{\infty} d\omega \, J(\omega) \left[\coth \frac{\hbar \omega \beta}{2} \cos \omega t - i \sin \omega t \right]$

weight function

thermal Green's function of a single harm. oscillator

Simplest case: Ohmic bath: $J(\omega) = \mathcal{M} \gamma \omega \; e^{-\omega/\omega_c}$

Damping becomes Markovian: $\gamma(t-s) = 2\gamma \delta(t-s)$

Path integral approach to open quantum systems

Bath d.o.f. not under control & not of interest: average over them:

Reduced density operator in system Hilbert space: $\rho(t) \equiv \mathrm{tr}_{\mathrm{B}} \mathbf{W}(\mathrm{t})$

$$\rho(q_{\mathrm{f}}, q'_{\mathrm{f}}, t) = \prod_{j=1}^{\mathcal{N}} \int dx_{j,\mathrm{f}} \, \langle q_{\mathrm{f}} \boldsymbol{x}_{\mathrm{f}} | \mathbf{W}(t) | q'_{\mathrm{f}} \boldsymbol{x}_{\mathrm{f}} \rangle$$

$$= \int dq_{\mathrm{i}} \int dq'_{\mathrm{i}} \, \mathcal{G}(q_{\mathrm{f}}, q'_{\mathrm{f}}, t; q_{\mathrm{i}}, q'_{\mathrm{i}}, t_0) \rho_{\mathrm{S}}(q_{\mathrm{i}}, q'_{\mathrm{i}}, t_0)$$

possible, since action quadratic: Gaussian integral

$$\mathcal{G}(q_{\mathrm{f}}, q'_{\mathrm{f}}, t; q_{\mathrm{i}}, q'_{\mathrm{i}}, t_0) = \int_{q(t_0)=q_{\mathrm{i}}}^{q(t)=q_{\mathrm{f}}} \mathcal{D}q \int_{q'(t_0)=q'_{\mathrm{i}}}^{q'(t)=q'_{\mathrm{f}}} \mathcal{D}q' \exp\left\{ \frac{i}{\hbar} \left(S_{\mathrm{S}}[q] - S_{\mathrm{S}}[q'] \right) \right\} \mathcal{F}_{\mathrm{FV}}[q, q']$$

Feynman-Vernon influence functional:

$$\mathcal{F}_{\mathrm{FV}}[q, q'] = e^{-\frac{1}{\hbar} \phi_{\mathrm{FV}}[q, q']}$$

Feynman-Vernon influence functional

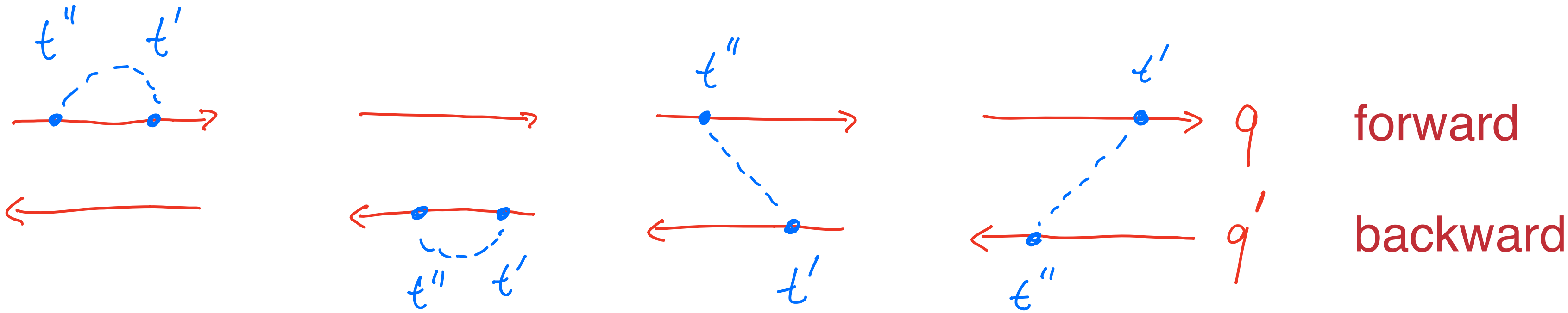
$$\mathcal{F}_{\mathrm{FV}}[q,q'] = e^{-\frac{1}{\hbar}\phi_{\mathrm{FV}}[q,q']}$$

with

$$\phi_{\mathrm{FV}}[q,q'] = \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \{q(t') - q'(t')\}\{\eta(t'-t'')q(t'') - \eta^*(t'-t'')q'(t'')\}$$

with integral kernel

$$\eta(t) = L(t) + i\delta(t)\frac{2}{\pi}\int_0^\infty d\omega \frac{J(\omega)}{\omega}$$



Consequences of bath fluctuations:

- time correlations between paths of system dynamics
- complex correlation function

Quasiadiabatic propagator path-integral

In general, we need numerical approach for exact solutions

Here: Quasiadiabatic propagator path integral (QUAPI)

N. Makri, J. Math. Phys. **36**, 2430 (1995)

- numerically exact method
- for all forms of spectral density (no restriction in principle)
- for any finite temperature bath
- system can be general
- driven quantum systems
- latest boost: tensor-network formulation TEMPO

Limitations / drawbacks:

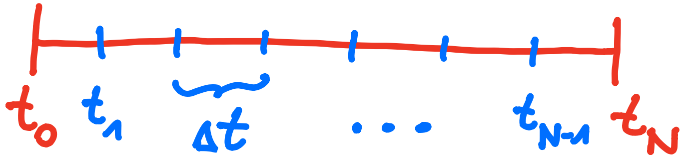
- not too large system Hilbert space dimension, M up to 12-15 or so
- not for zero temperature case (in principle)

General idea: deterministic summation of dissipative real-time path integral

Quasiadiabatic propagator path-integral

N. Makri, J. Math. Phys. **36**, 2430 (1995)

Time discretization (as usual)
=> Short-time propagators



QUAPI in 3 steps:

$$\mathbf{H}(t) = \mathbf{H}_{\mathrm{S}}(t) + \mathbf{H}_{\mathrm{B}}$$

contains $\mathbf{H}_{\mathrm{B}} + \mathbf{H}_{\mathrm{SB}}$

1. Step: Symmetric Trotter splitting of short-time propagator:

$$\mathbf{U}(t_{k+1}, t_k) \approx \exp(-i\mathbf{H}_{\mathrm{B}}\Delta t/2\hbar)\mathbf{U}_{\mathrm{S}}(t_{k+1}, t_k)\exp(-i\mathbf{H}_{\mathrm{B}}\Delta t/2\hbar)$$

General time-ordered system propagator

$$\mathbf{U}_{\mathrm{S}}(t_{k+1}, t_k) = \mathcal{T}\exp\left\{-\frac{i}{\hbar}\int_{t_k}^{t_{k+1}} dt'\,\mathbf{H}_{\mathrm{S}}(t')\right\}$$

Trotter error:

$$\sim \mathcal{O}([\mathbf{H}_{\mathrm{B}}, [\mathbf{H}_{\mathrm{S}}, \mathbf{H}_{\mathrm{B}}]]\Delta t^3)$$

Quasiadiabatic propagator path-integral

N. Makri, J. Math. Phys. **36**, 2430 (1995)

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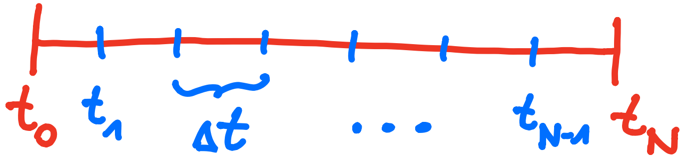


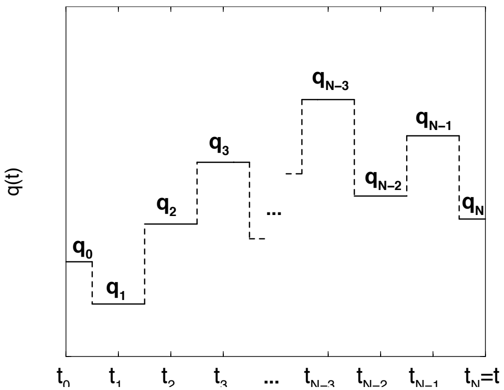
$$\mathbf{H}(t) = \mathbf{H}_\mathrm{S}(t) + \mathbf{H}_\mathrm{B}$$

contains $\mathbf{H}_\mathrm{B} + \mathbf{H}_\mathrm{SB}$

1. Step: Symmetric Trotter splitting of short-time propagator:

Short-time propagator factorizes:

$$\langle q\,\Pi_j x_j|\mathbf{U}(t_{k+1},t_k)|q'\,\Pi_j x_j'\rangle \approx \langle q|\mathbf{U}_\mathrm{S}(t_{k+1},t_k)|q'\rangle \prod_{j=1}^{\mathcal{N}} \langle x_j|e^{-i\mathbf{H}_j(q)\Delta t/2\hbar}e^{-i\mathbf{H}_j(q')\Delta t/2\hbar}|x_j'\rangle$$



System coordinate treated quasi-adiabatically
-> QUAPI

Quasiadiabatic propagator path-integral

N. Makri, J. Math. Phys. **36**, 2430 (1995)

Combine to full propagator from initial to final time (use completeness…)
& carry out integration over bath d.o.f. (partial trace):

Reduced density operator at time t:

$$\rho(q_{\mathrm{f}}, q'_{\mathrm{f}}; t) = \int dq_0 \ldots \int dq_N \int dq'_0 \ldots \int dq'_N \, \delta(q'_{\mathrm{f}} - q'_N)\, \delta(q_{\mathrm{f}} - q_N)$$
$$\times \langle q_N | \mathbf{U}_{\mathrm{S}}(t, t-\Delta t) | q_{N-1} \rangle \ldots \langle q_1 | \mathbf{U}_{\mathrm{S}}(t_0 + \Delta t, t_0) | q_0 \rangle$$
$$\times \langle q_0 | \rho_{\mathrm{S}}(t_0) | q'_0 \rangle \langle q'_0 | \mathbf{U}_{\mathrm{S}}^{-1}(t_0 + \Delta t, t_0) | q'_1 \rangle \ldots \langle q'_{N-1} | \mathbf{U}_{\mathrm{S}}^{-1}(t, t - \Delta t) | q'_N \rangle$$
$$\times \mathcal{F}_{FV}^{(N)}(q_0, q'_0, \ldots, q_N, q'_N)$$

discrete Feynman-Vernon influence functional:

$$\mathcal{F}_{FV}^{(N)}(q_0, \ldots, q'_N) = \exp\left\{ -\frac{1}{\hbar} \sum_{k=0}^{N} \sum_{k'=0}^{k} [q_k - q'_k][\eta_{kk'} q_{k'} - \eta^*_{kk'} q'_{k'}] \right\} .$$

$$\eta_{kk'} = \eta(t_k - t'_k)$$

Remember:

$$\eta(t) = L(t) + i\delta(t) \frac{2}{\pi} \int_0^\infty d\omega \frac{J(\omega)}{\omega}$$

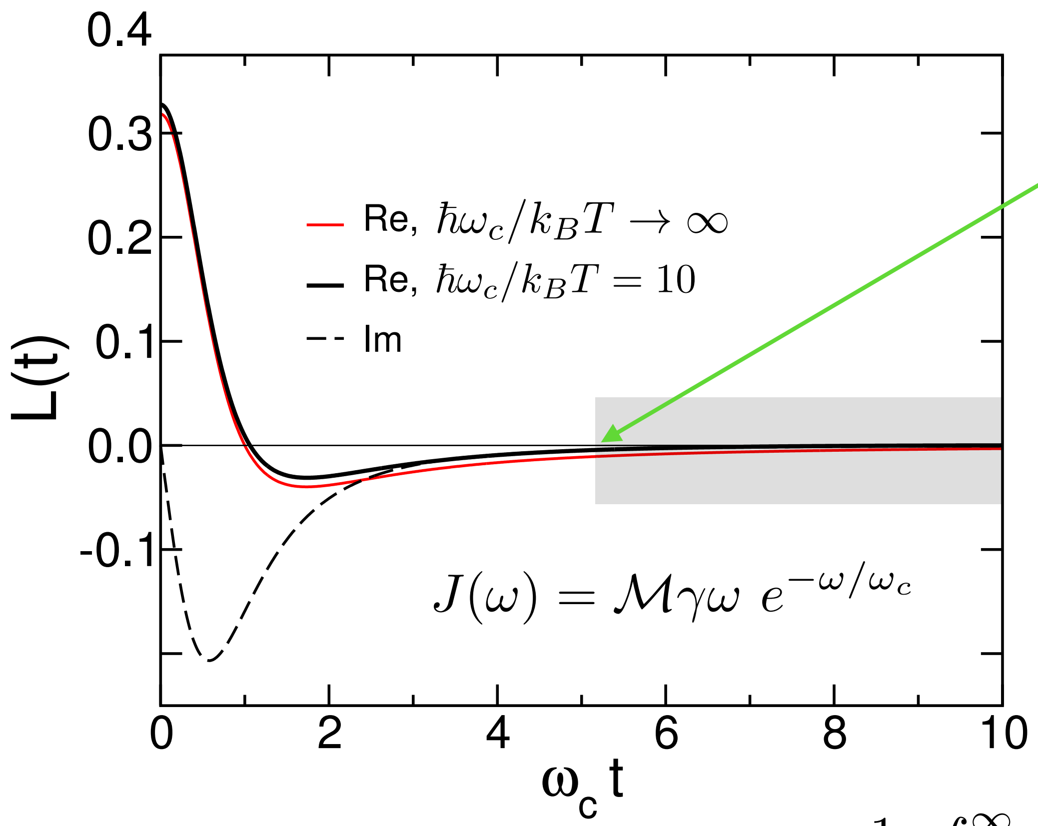
Quasiadiabatic propagator path-integral

N. Makri, J. Math. Phys. **36**, 2430 (1995)

2. Step: Cut memory when it is negligible:

For any finite temperature: memory decays exponentially, i.e., there exists a memory time scale!

$$\tau_{\text{mem}} = K \Delta t$$



Idea: neglect memory when it is small enough for convergence!

Remember: $L(t) = \frac{1}{\pi}\int_0^\infty d\omega\, J(\omega)\left[\coth\frac{\hbar\omega\beta}{2}\cos\omega t - i\sin\omega t\right]$

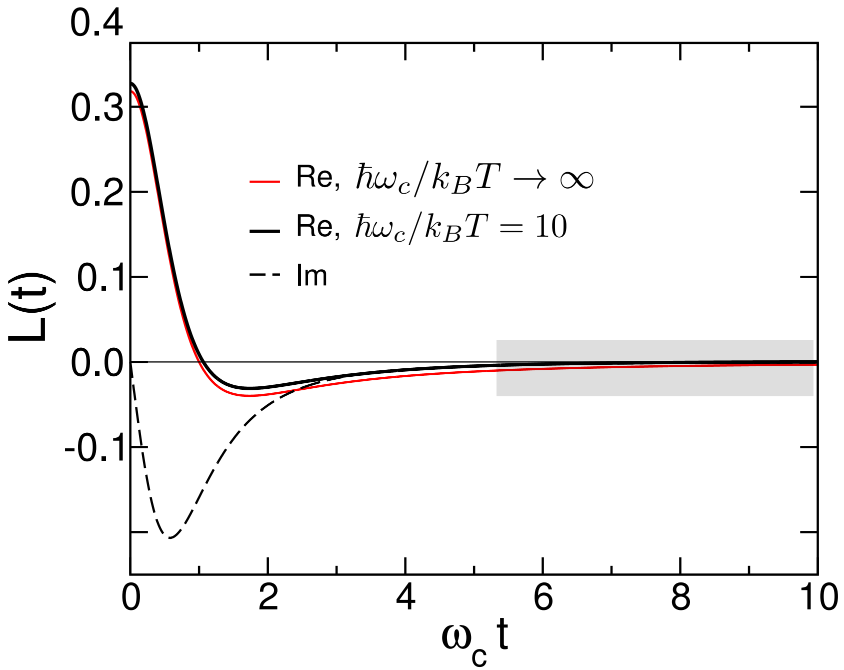
Quasiadiabatic propagator path-integral

N. Makri, J. Math. Phys. **36**, 2430 (1995)

2. Step: Cut memory when it is negligible:

$$\tau_{\text{mem}} = K\Delta t$$

$$\mathcal{F}_{FV}^{(N)}(q_0, ..., q_N') \approx \prod_{k=0}^{N} \prod_{k'=0}^{\min\{N,K\}} \exp\left\{-\frac{1}{\hbar}[q_k - q_k'][\eta_{kk'}q_{k'} - \eta_{kk'}^* q_{k'}']\right\}$$



in practice: increase K until numerical convergence is established

Remember: $\mathcal{F}_{FV}^{(N)}(q_0, ..., q_N') = \exp\left\{-\frac{1}{\hbar}\sum_{k=0}^{N}\sum_{k'=0}^{k}[q_k - q_k'][\eta_{kk'}q_{k'} - \eta_{kk'}^* q_{k'}']\right\}$.

Quasiadiabatic propagator path-integral

N. Makri, J. Math. Phys. **36**, 2430 (1995)

Iterative tensor multiplication scheme:

$$\rho(q, q', t) \equiv \rho_k(q_k, q'_k) \quad \Rightarrow \quad A_k(q_k, ..., q'_{k+K-1})$$

reduced density matrix (local in time) → reduced density tensor (depends on memory)

propagate numerically: iteration:

$$A_{k+1}(q_{k+1}, ..., q'_{k+K}) = \int dq_k \int dq_{k'} \Lambda_k(q_k, ..., q'_{k+K}) \, A_k(q_k, ..., q'_{k+K-1})$$

with propagating tensor:

$$\Lambda_k(q_k, ..., q'_{k+K}) = \langle q_{k+1} | \mathbf{U}_\mathrm{S}(t_{k+1}, t_k) | q_k \rangle \langle q'_k | \mathbf{U}_\mathrm{S}^{-1}(t_{k+1}, t_k) | q'_{k+1} \rangle \prod_{k'=0}^{K} \exp\left\{ -\frac{1}{\hbar} [q_k - q'_k][\eta_{kk'} q_{k'} - \eta^*_{kk'} q'_{k'}] \right\}$$

At final time: $\rho(q_f, q'_f, t) = A_N(q_f, q'_f, \hat{q}, ..., \hat{q}) \exp\left\{ -\frac{1}{\hbar} [q_f - q'_f][\eta_{NN} q_f - \eta^*_{NN} q'_f] \right\}$

Quasiadiabatic propagator path-integral

N. Makri, J. Math. Phys. **36**, 2430 (1995)

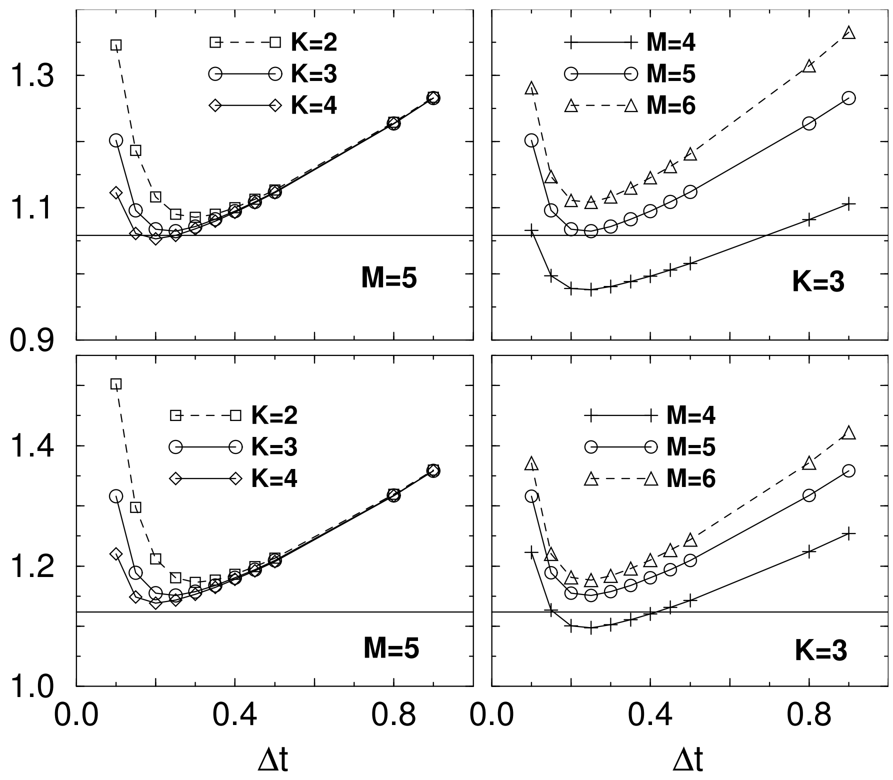
3. Step: Discrete variable representation

$$\int dq_k \int dq_{k'} \ldots \quad \Rightarrow \quad \sum_{m_k=1}^{M} \sum_{m'_k=1}^{M} \cdots$$

dimension of system Hilbert space

continuous integration in coordinate space → discrete summation in eigenspace of system-bath coupling operator

$\sigma_{qq}(\infty)$



Careful check for convergence:

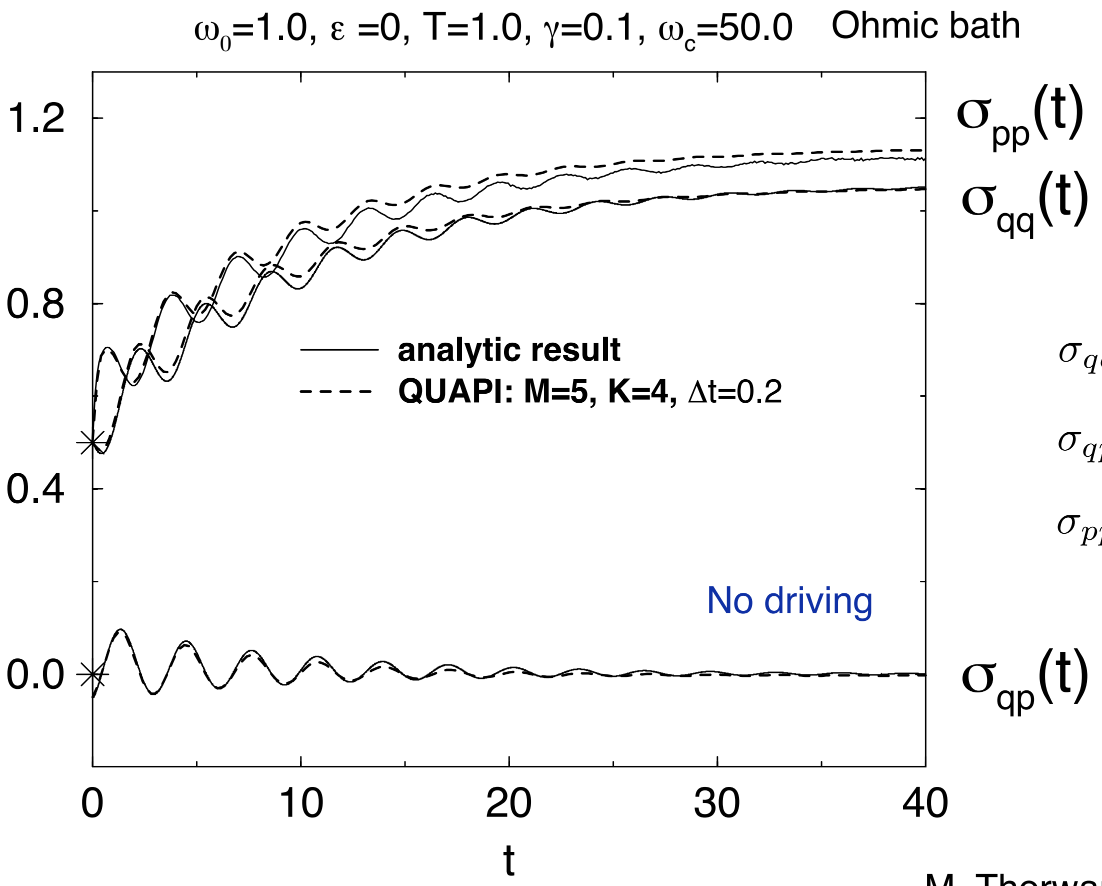
- Trotter increment as small as possible
- memory time as large as possible
- optimum in between

M. Thorwart, P. Reimann, P. Hänggi, Rev. E **62**, 5808 (2000)

QUAPI: Verification & tests

Parametrically driven quantum dissipative harmonic oscillator

$$\mathbf{H}_\mathrm{S}(t) = \frac{\mathbf{p}^2}{2\mathcal{M}} + \frac{\mathcal{M}}{2}[\omega_0^2 + \epsilon\cos\Omega t]\mathbf{q}^2$$



$$\sigma_{qq}(t) \equiv \langle \mathbf{q}^2(t)\rangle - \langle \mathbf{q}(t)\rangle^2$$

$$\sigma_{qp}(t) \equiv \frac{1}{2}\langle \mathbf{q}(t)\mathbf{p}(t) + \mathbf{p}(t)\mathbf{q}(t)\rangle - \langle \mathbf{q}(t)\rangle\langle \mathbf{p}(t)\rangle$$

$$\sigma_{pp}(t) \equiv \langle \mathbf{p}^2(t)\rangle - \langle \mathbf{p}(t)\rangle^2$$

M. Thorwart, P. Reimann, P. Hänggi, Rev. E **62**, 5808 (2000)

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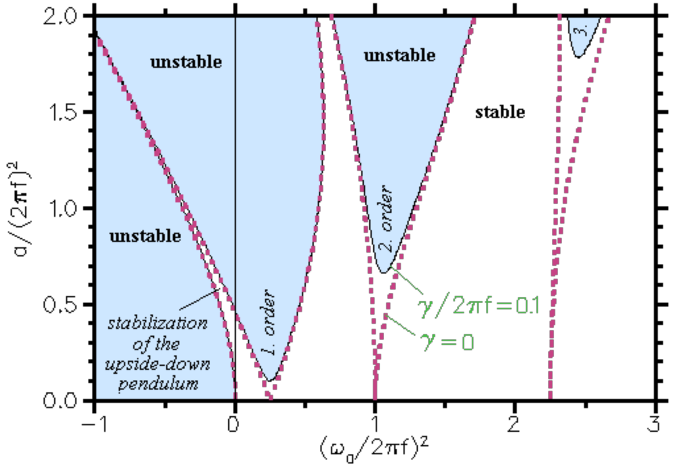
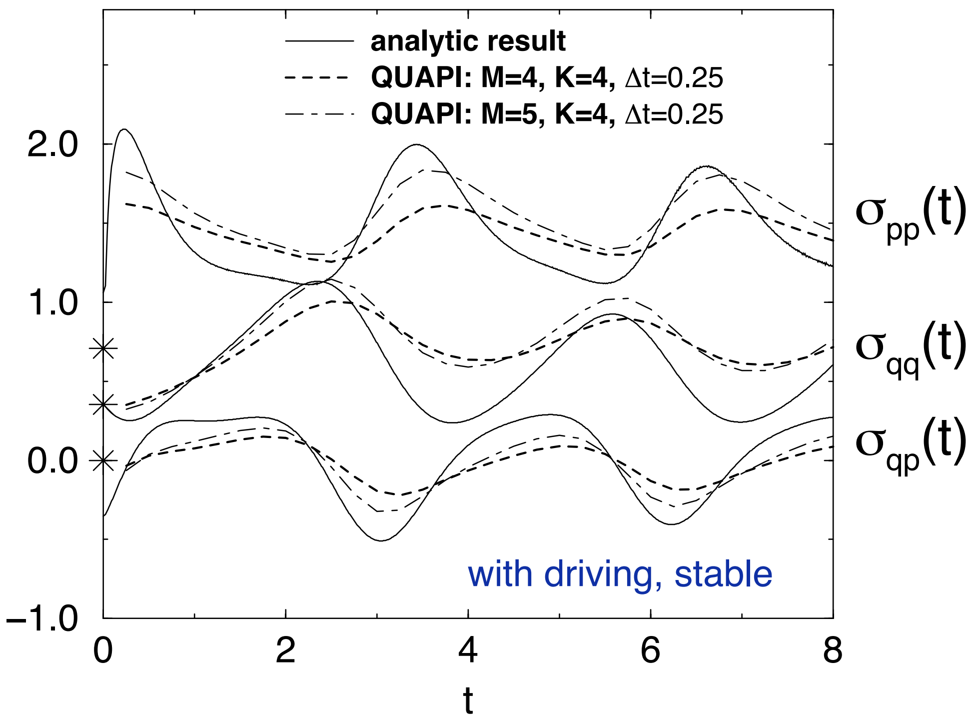


ω_0=1.0, ε =0.5, T=0.1, γ=1.0, ω_c=50.0 Ohmic bath



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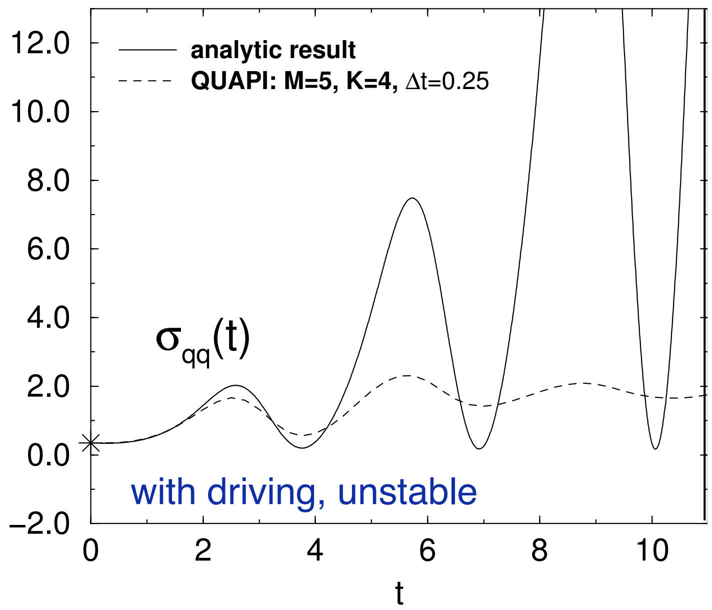


M. Thorwart, P. Reimann, P. Hänggi, Rev. E **62**, 5808 (2000)

Recent developments

1) Small Matrix decomposition of the Path Integral (SMatPI):

N. Makri, J. Chem. Phys. 152, 041104 (2020)

- eliminates the large memory requirements of the iterative QUAPI while introducing an approximation that is small compared to the memory cutoff

2) Extended SMatPI:

N. Makri, J. Chem. Theory Comput 17, 1 (2021)

- incorporates some additional long-range influence functional terms to SMatPI at essentially no computational cost

3) QUAPI as a tensor network: TEMPO

A. Strathearn, P. Kirton, D. Kilda, J. Keeling & B. W. Lovett, Nature Commun. 9, 3322 (2018)

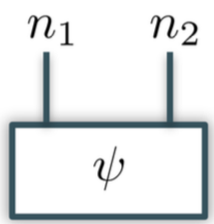
- general idea:
  TEMPO compresses the history of a dissipative single particle immersed in a heat bath into a matrix product state („DMRG in time“)

Basics of matrix product states

Consider general state in a two-body Hamiltonian:

$$|\psi\rangle = \sum_{n_1,n_2} |n_1,n_2\rangle \langle n_1,n_2 \,|\, \psi\rangle =: \sum_{n_1,n_2} \psi^{n_1 n_2} |n_1,n_2\rangle$$

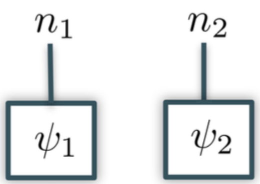
Graphical representation of coefficient matrix:



rank-2 „tensor“

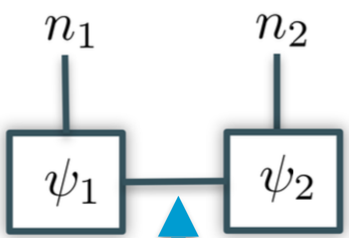
If state is not an entangled state:

$$\psi^{n_1 n_2} = \psi_1^{n_1} \psi_2^{n_2}$$



In general: matrix product state representation:

$$\psi^{n_1 n_2} = \sum_i (\psi_1)_i^{n_1} (\psi_2)_i^{n_2}$$



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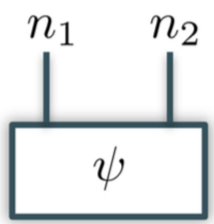

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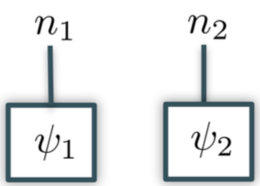

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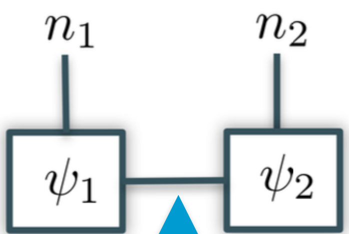


Singular-value decomposition:

$$\psi^{n_1 n_2} = \sum_{i=1}^{\mathrm{rank}(\psi^{n_1 n_2})} L_i^{n_1} \sigma_i R_i^{n_2}$$

$$(\psi_1)_i^{n_1} = L_i^{n_1} \sigma_i$$

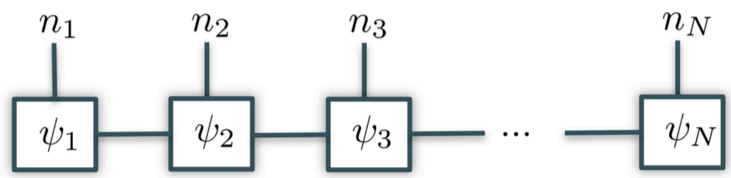
$$(\psi_2)_i^{n_2} = R_i^{n_2}$$

Basics of matrix product states

General state in an N-body Hamiltonian:

$$|\psi\rangle = \sum_{n_1,n_2,n_3,\ldots,n_N} \psi^{n_1 n_2 n_3 \ldots n_N} |n_1, n_2, n_3, \ldots, n_N\rangle$$

$$\psi^{n_1 n_2 n_3 \ldots n_N} = \sum_{i} (\psi_1)^{n_1}_{i_1} (\psi_2)^{n_2}_{i_1 i_2} (\psi_3)^{n_3}_{i_2 i_3} \cdots (\psi_N)^{n_N}_{i_{N-1}}$$



Advantage:

MPS is a rank-N tensor, while consisting of only rank-3 tensors

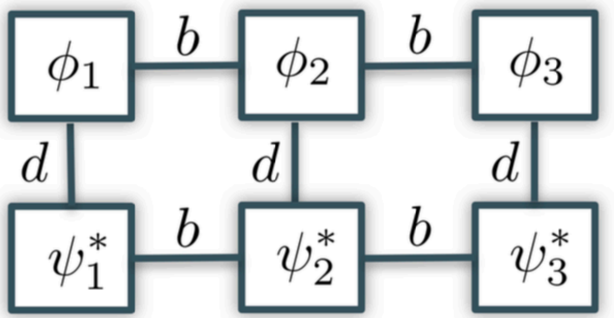
object no longer scales exponentially in N, when not all states are fully entangled (as is often the case)

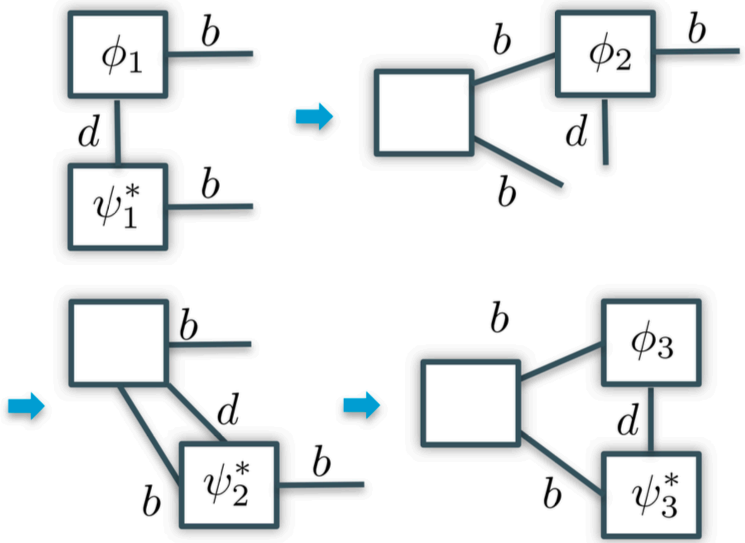
Strong computational advantage

Basics of matrix product states

Contraction:

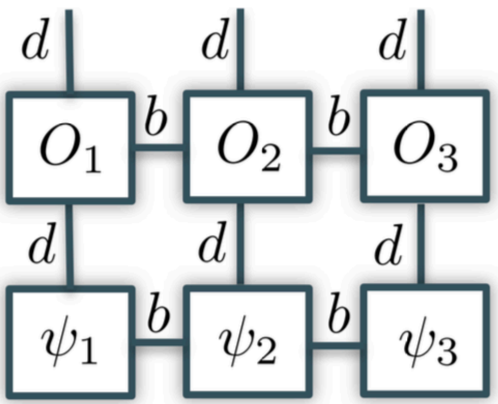
Scalar product $\langle \psi | \phi \rangle$



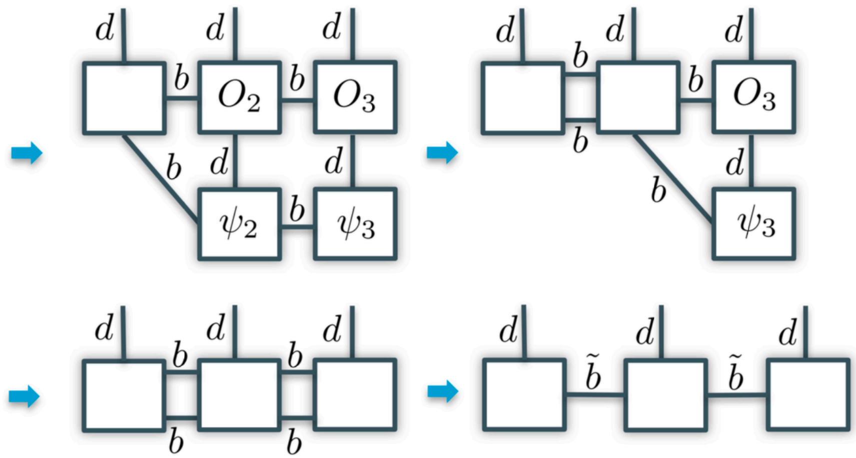


Operators:

Matrix product operator $\hat{O}$ acting on a matrix product state $|\psi\rangle$



Contraction:

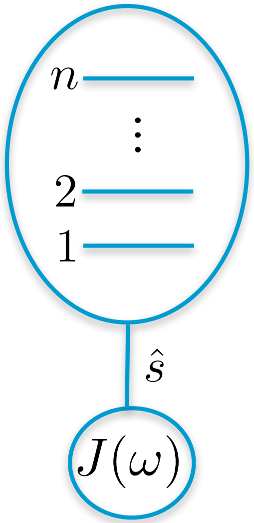


Tensor network formulation: TEMPO

Slight change of notation

$$\hat{H} = \hat{H}_S + \hat{H}_{\text{env}} = \hat{H}_S + \sum_j \left[\frac{\hat{p}_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 \left(\hat{x}_j - \frac{c_j \hat{s}}{m_j \omega_j^2} \right)^2 \right] \qquad \hbar = 1$$

$$\hat{H}_S = \sum_{i,j=1}^{n} h_{ij} \left| s_i \right\rangle \left\langle s_j \right| \qquad \hat{s} = \sum_{i=1}^{n} s_i \left| s_i \right\rangle \left\langle s_i \right|$$



spectral density: $J(\omega) = \frac{\pi}{2} \sum_j \frac{c_j^2}{m_j \omega_j} \delta(\omega - \omega_j).$

Tensor network formulation: TEMPO

Remember: QUAPI: reduced density matrix

$$\left\langle s_{i_N^+} \middle| \rho_S(t) \middle| s_{i_N^-} \right\rangle = \left\langle s_{i_N^+} \middle| \mathrm{Tr}_{\mathrm{env}} \left(e^{-i\hat{H}t} \rho(0) e^{i\hat{H}t} \right) \middle| s_{i_N^-} \right\rangle$$

$$t = N \cdot \Delta t \quad \overset{[2]}{=} \sum_{i_0^\pm, \ldots, i_{N-1}^\pm = 1}^{n} G_{i_N^\pm i_{N-1}^\pm} \cdots G_{i_1^\pm i_0^\pm} \left\langle s_{i_0^+} \middle| \rho_S(0) \middle| s_{i_0^-} \right\rangle \prod_{k=0}^{N} \prod_{k'=0}^{k} F^{(kk')}_{i_k^\pm i_{k'}^\pm} + \mathcal{O}\left(\Delta t^2\right)$$

System propagator: $$G_{i_{k+1}^\pm, i_k^\pm} = \left\langle s_{i_{k+1}^+} \middle| e^{-iH_S \Delta t} \middle| s_{i_k^+} \right\rangle \left\langle s_{i_k^-} \middle| e^{iH_S \Delta t} \middle| s_{i_{k+1}^-} \right\rangle$$

Bath influence: $$F^{(kk')}_{i_k^\pm i_{k'}^\pm} = \exp\left[-\left(s_{i_k^+} - s_{i_k^-}\right) \left(\eta_{kk'} s_{i_{k'}^+} - \eta^*_{kk'} s_{i_{k'}^-} \right) \right]$$

$$\eta_{kk'} \approx \Delta t^2 L((k-k')\Delta t) \quad \text{for } k \neq k'$$

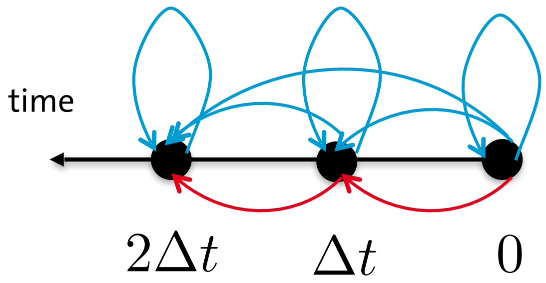
$$L(t) = \frac{1}{\pi} \int_0^\infty \mathrm{d}\omega J(\omega) \left[\coth\left(\frac{\omega \beta}{2} \right) \cos(\omega t) - i \sin(\omega t) \right]$$

- → numerically exact
- → arbitrary spectral density

[2] N. Makri and D. E. Makarov, J. Chem. Phys. 102, 4611 (1995).

Tensor network formulation: TEMPO

Notation: $\alpha := i^{\pm}$



Consider example $N = 2$ time steps

$$\rho_S(2\Delta t)_{\alpha_2} = \sum_{\alpha_0,\alpha_1=1}^{n^2} \underline{G_{\alpha_2\alpha_1} G_{\alpha_1\alpha_0}} \rho_{\alpha_0} \underline{F^{(22)}_{\alpha_2\alpha_2} F^{(21)}_{\alpha_2\alpha_1} F^{(20)}_{\alpha_2\alpha_0} F^{(11)}_{\alpha_1\alpha_1} F^{(10)}_{\alpha_1\alpha_0} F^{(00)}_{\alpha_0\alpha_0}}$$

➡ absorb system propagator:

$$I_{\alpha_{k_1}\alpha_{k_2}} := \begin{cases} G_{\alpha_{k_1}\alpha_{k_2}} F^{(k_1 k_2)}_{\alpha_{k_1}\alpha_{k_2}} & \text{if } k_1 - k_2 = 1 \\ F^{(k_1 k_2)}_{\alpha_{k_1}\alpha_{k_2}} & \text{else} \end{cases}$$

➡ $$\boxed{\rho_S(N\Delta t)_{\alpha_N} = \sum_{\alpha_0,\ldots,\alpha_{N-1}=1}^{n^2} \rho_{\alpha_0} \prod_{k=0}^{N} \prod_{k'=0}^{k} I_{\alpha_k \alpha_{k'}}}$$

A. Strathearn, P. Kirton, D. Kilda, J. Keeling & B. W. Lovett, Nature Commun. 9, 3322 (2018)

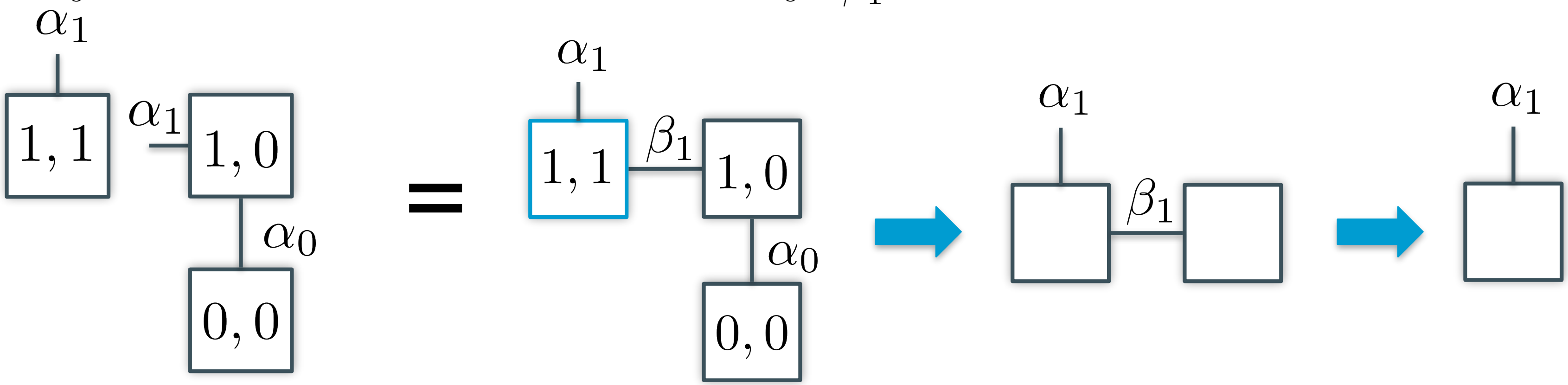
Tensor network formulation: TEMPO

$$\rho_S(N\Delta t)_{\alpha_N} = \sum_{\alpha_0,\ldots,\alpha_{N-1}=1}^{n^2} \rho_{\alpha_0} \prod_{k=0}^{N} \prod_{k'=0}^{k} I_{\alpha_k \alpha_{k'}}$$

Consider $N = 1:$

Key point: use Kronnecker

$$\rho_S(\Delta t)_{\alpha_1} = \sum_{\alpha_0} I_{\alpha_1\alpha_1} I_{\alpha_1\alpha_0} I_{\alpha_0\alpha_0} \rho_{\alpha_0} = \sum_{\alpha_0}\sum_{\beta_1} \delta_{\alpha_1\beta_1} I_{\alpha_1\alpha_1} I_{\alpha_1\alpha_0} I_{\alpha_0\alpha_0} \rho_{\alpha_0}$$

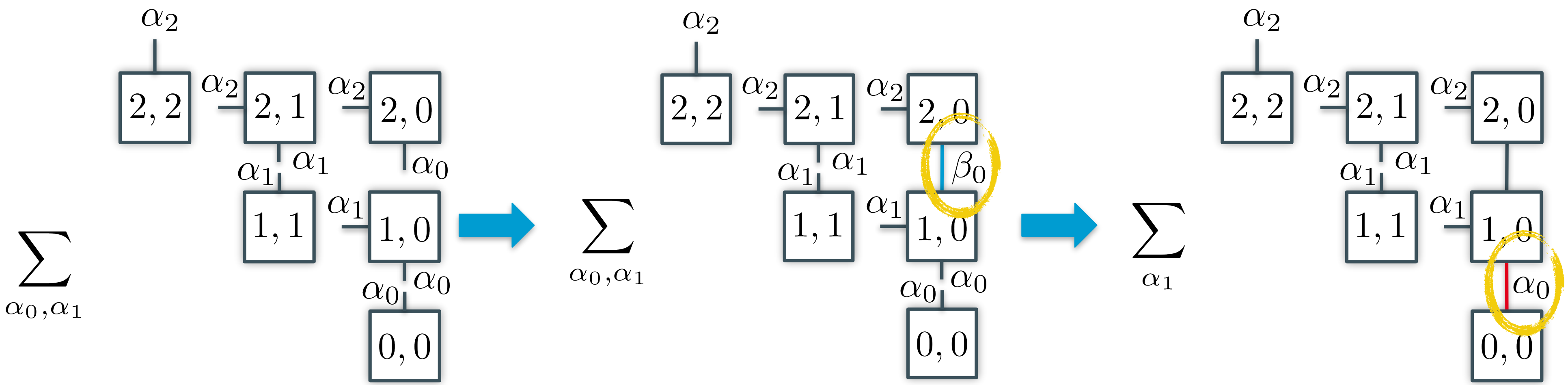


A. Strathearn, P. Kirton, D. Kilda, J. Keeling & B. W. Lovett, Nature Commun. 9, 3322 (2018)

Tensor network formulation: TEMPO

Consider $N = 2$:

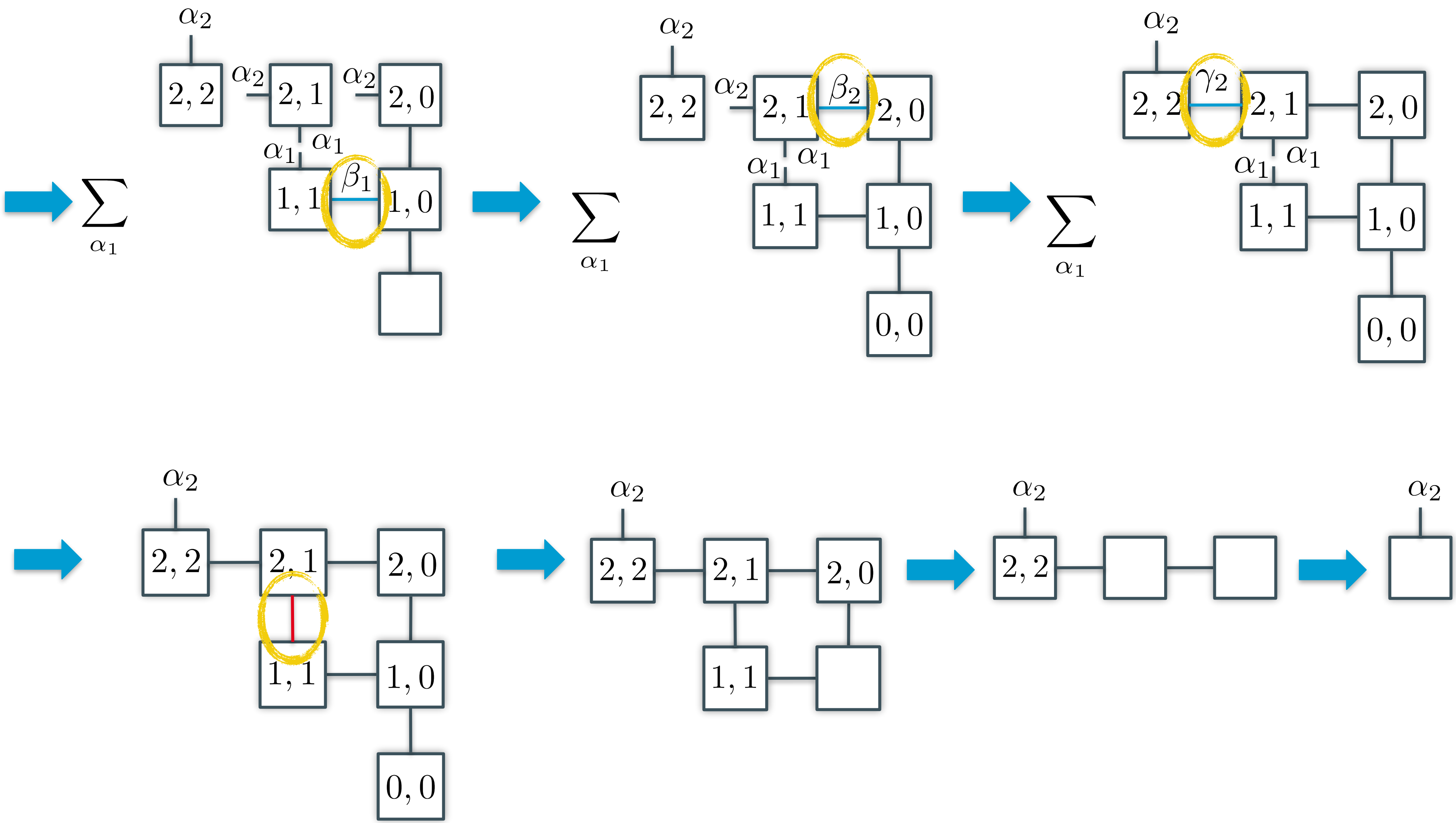
$$\rho_S(2\Delta t)_{\alpha_2} = \sum_{\alpha_0,\alpha_1} I_{\alpha_2\alpha_2} I_{\alpha_2\alpha_1} I_{\alpha_2\alpha_0} I_{\alpha_1\alpha_1} I_{\alpha_1\alpha_0} I_{\alpha_0\alpha_0} \rho_{\alpha_0}$$



A. Strathearn, P. Kirton, D. Kilda, J. Keeling & B. W. Lovett, Nature Commun. 9, 3322 (2018)

Tensor network formulation: TEMPO

Consider $N = 2$:

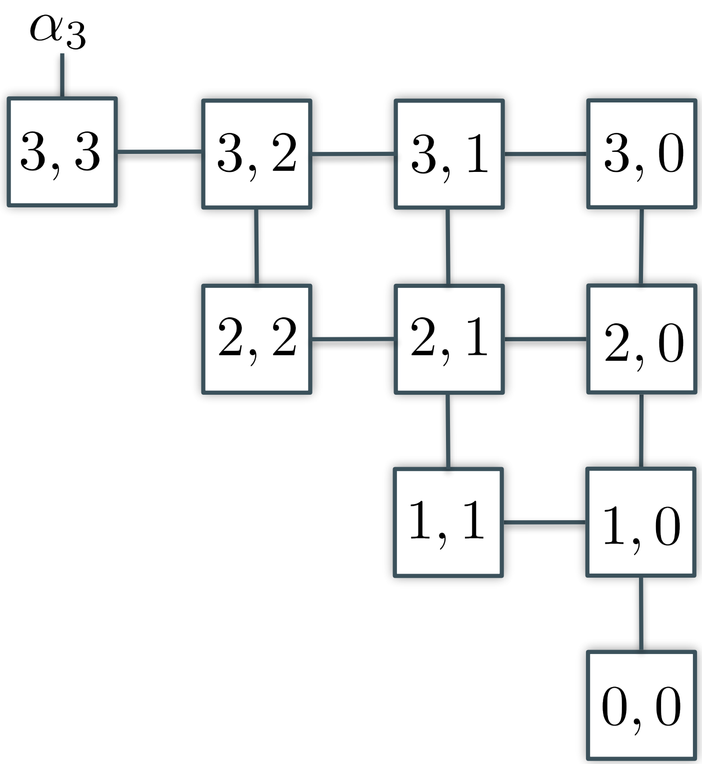


A. Strathearn, P. Kirton, D. Kilda, J. Keeling & B. W. Lovett, Nature Commun. 9, 3322 (2018)

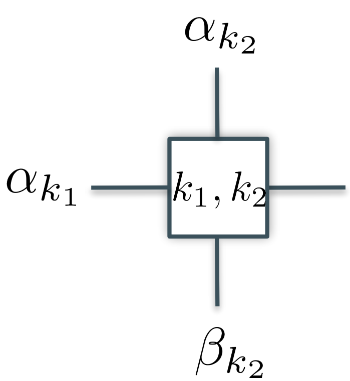
Tensor network formulation: TEMPO

Consider $N = 3$:

$$\rho_S(3\Delta t)_{\alpha_3} =$$



where



$$= \delta_{\alpha_{k_1}\beta_{k_1}}\delta_{\alpha_{k_2}\beta_{k_2}} I_{\alpha_{k_1}\alpha_{k_2}}$$

A. Strathearn, P. Kirton, D. Kilda, J. Keeling & B. W. Lovett, Nature Commun. 9, 3322 (2018)

Tensor network formulation: TEMPO

Decisive advantage of TEMPO:

- Substantially many, many more memory time steps can be taken into account

- Typical for QUAPI:
  up to 18 to 20 memory time steps for a qubit-system

- TEMPO:
  several hundred memory time steps are possible

- extends the range of applicability of the method to very hard extrem non-Markovian cases

Benchmark test: Qubit + oscillator

$$\hat{H} = \hat{H}_{\mathrm{S}} + \hat{H}_{\mathrm{int}} + \hat{H}_{\mathrm{osc}} = \frac{\Omega}{2}\hat{\sigma}_x - \frac{g}{2}\hat{\sigma}_z\left(\hat{a} + \hat{a}^\dagger\right) + \nu\hat{a}^\dagger\hat{a}$$

Worst case scenario for TEMPO: no compact tensor to compress memory $\Omega = g = \nu$

initial condition:

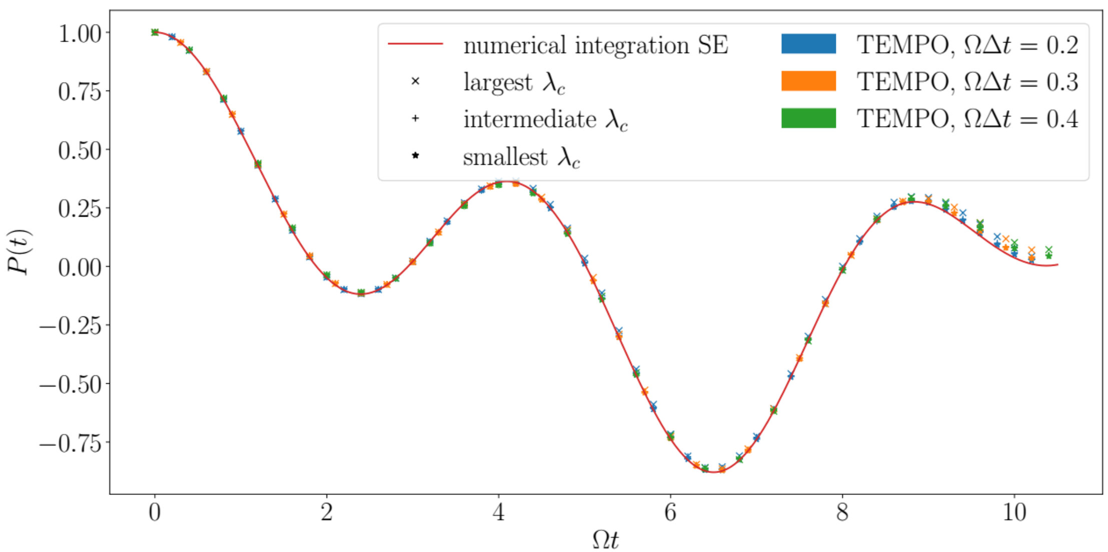
$\rho_S(0) = |\uparrow\rangle$

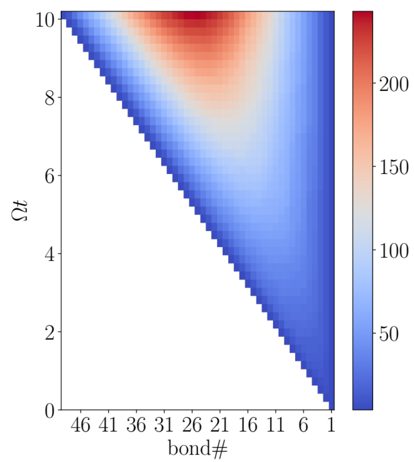
$\rho_{\mathrm{osc}}(0) = |0\rangle$

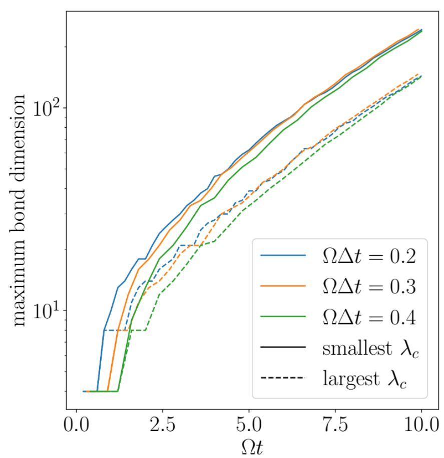
$\Rightarrow J(\omega) = \pi g^2 \delta(\omega - \nu) \Rightarrow L(t) = g^2 e^{-i\nu t}$

Two (controlled) approximations: time step Δt and singular value cutoff λ_c

polarization $P(t) := \langle\hat{\sigma}_z\rangle_t = \mathrm{Tr}\left(\hat{\sigma}_z \rho_S(t)\right)$







Examples & Applications

- dissipative quantum XOR gate
- Superconducting qubit coupled to a SQUID as readout device
- sub-Ohmic bath
- Quantum-1/f noise in superconducting qubits
- Superconducting qubits exposed to non-commuting baths

Dissipative quantum XOR gate

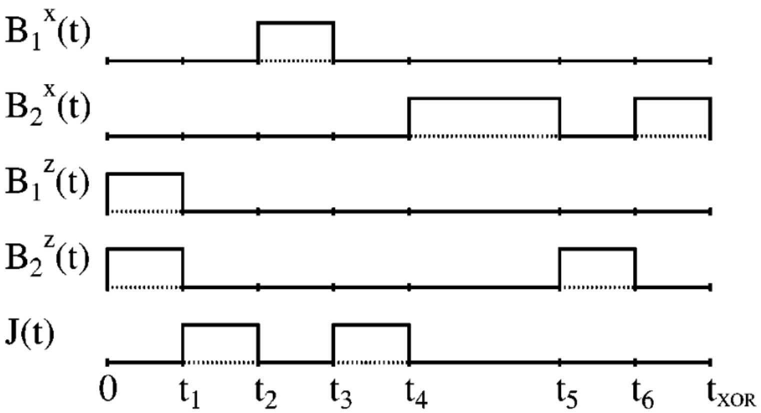
$$|00\rangle \quad |01\rangle \quad |10\rangle \quad |11\rangle$$

$$U_{\text{XOR}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Two coupled qubits:

$$H_{\text{XOR}}(t) = -\frac{\hbar}{2}\sum_{j=1}^{2} \vec{B}_j(t)\vec{\sigma}_j + \hbar \sum_{j \neq k} J(t)\,\sigma_j^+ \sigma_k^-$$

$$H_{\text{int}}^{x/z} = H_c^{x/z} \sum_{j=1}^{N} \kappa_j^{x/z} (a_j^+ + a_j)$$



Set	B^z	B^x	J	T	B^x/B^z	J/B^z	T/B^z	$t_{\text{XOR}}B^z$
I (Flux qubits)	0.5 K	50 mK	25 mK	25 mK	0.1	0.05	0.05	82(π/2)
II (Charge qubits)	1 K	100 mK	5 mK	50 mK	0.1	0.005	0.05	442(π/2)
III (Quantum-dot qubits)	1 meV	1 meV	0.05 meV	125 mK	1	0.05	0.01	46(π/2)

System-bath coupling: (Ohmic)

1) Bit flip errors:

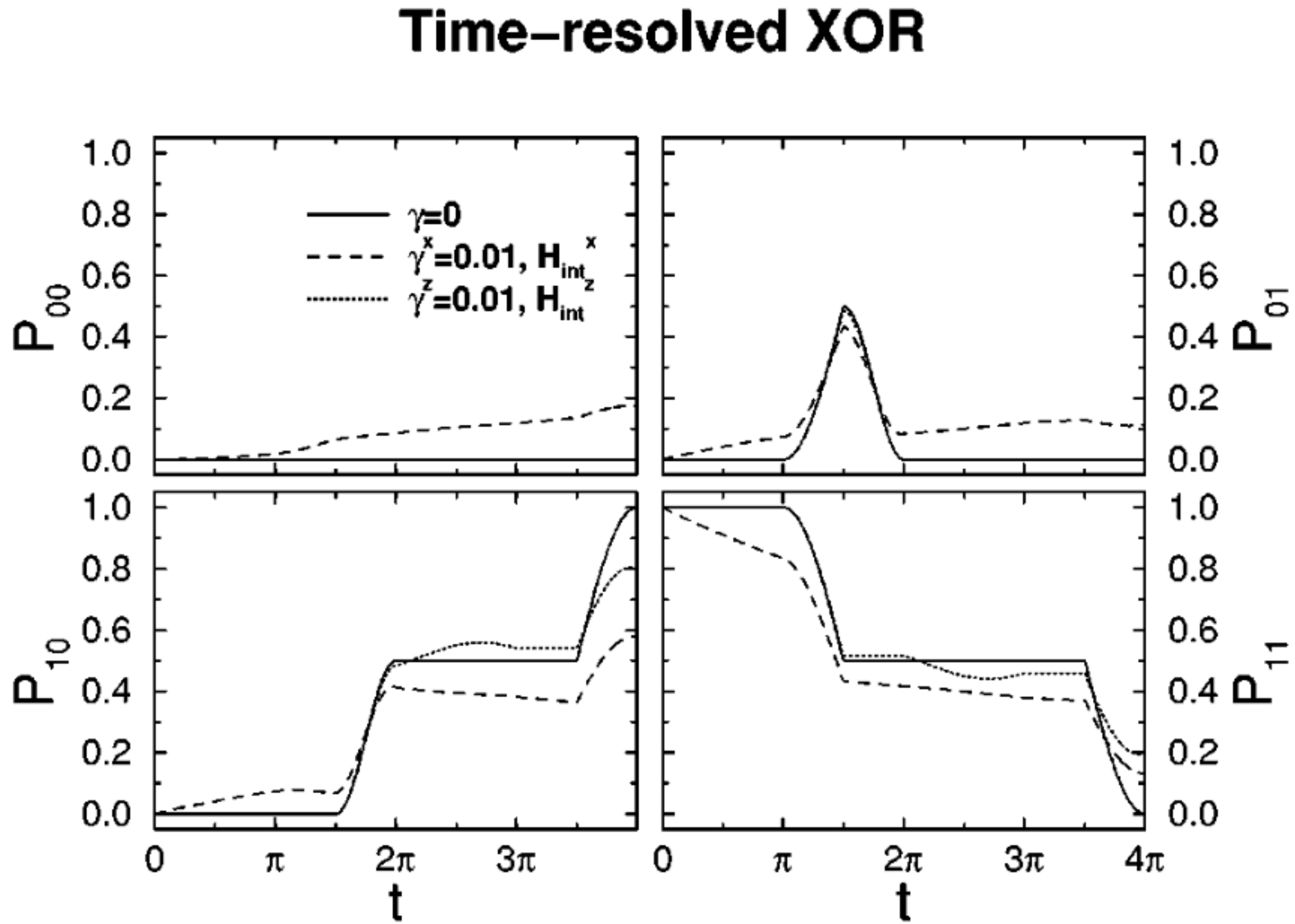
$$H_c^x = \frac{1}{2}(\sigma_1^x + \sigma_2^x) = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

2) Phase errors:

$$H_c^z = \frac{1}{2}(\sigma_1^z + \sigma_2^z) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

M. Thorwart, P. Hänggi, Phys. Rev. A **65**, 012309 (2000)

Dissipative quantum XOR gate



M. Thorwart, P. Hänggi, Phys. Rev. A **65**, 012309 (2000)

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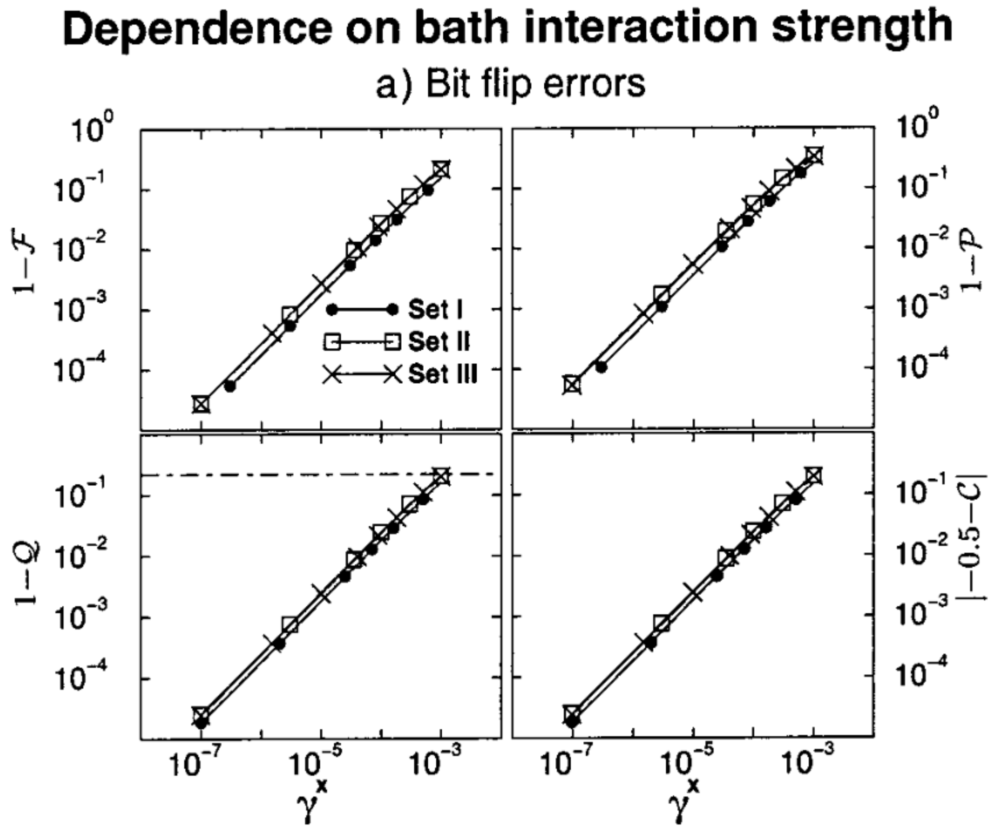
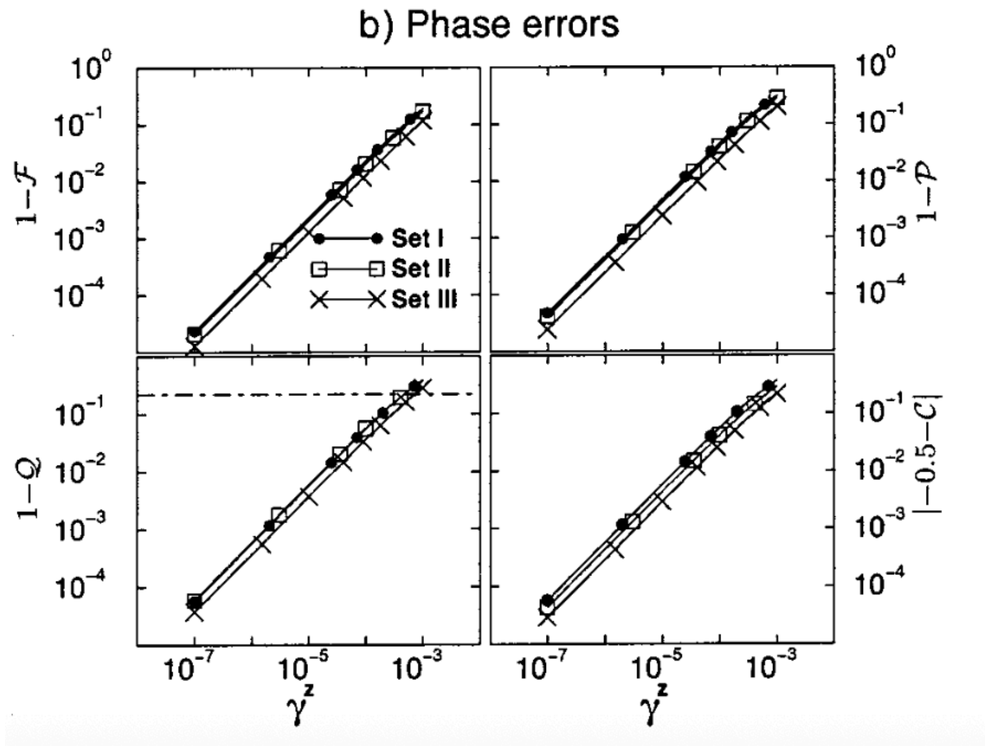
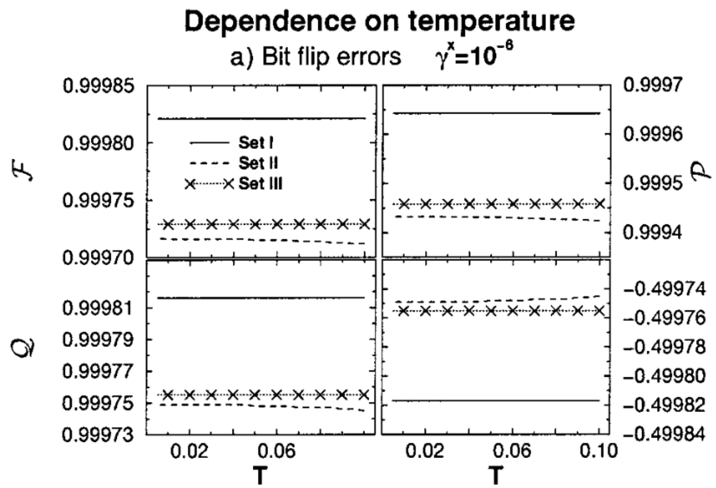






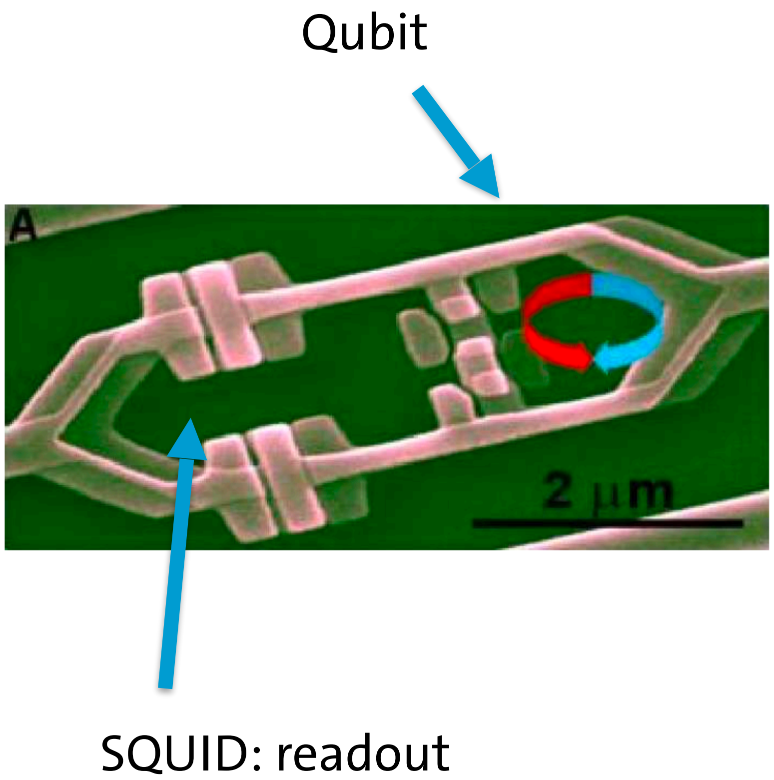
(similar for phase errors)

- decisive parameter: coupling strength
- temperature less crucial

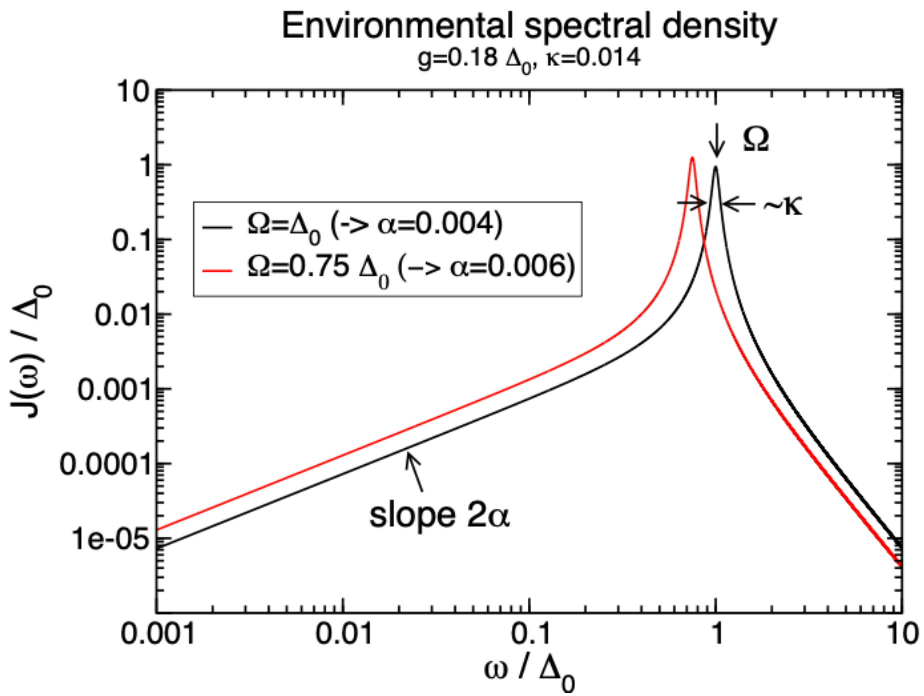
M. Thorwart, P. Hänggi, Phys. Rev. A **65**, 012309 (2000)

Superconducting qubit + readout

$$\tilde{H} = -\frac{\hbar\Delta_0}{2}\sigma_x - \frac{\hbar\varepsilon}{2}\sigma_z + \frac{1}{2}\sigma_z\hbar\sum_k \tilde{\lambda}_k(\tilde{b}_k^\dagger + \tilde{b}_k) + \sum_k \hbar\tilde{\omega}_k\tilde{b}_k^\dagger\tilde{b}_k$$



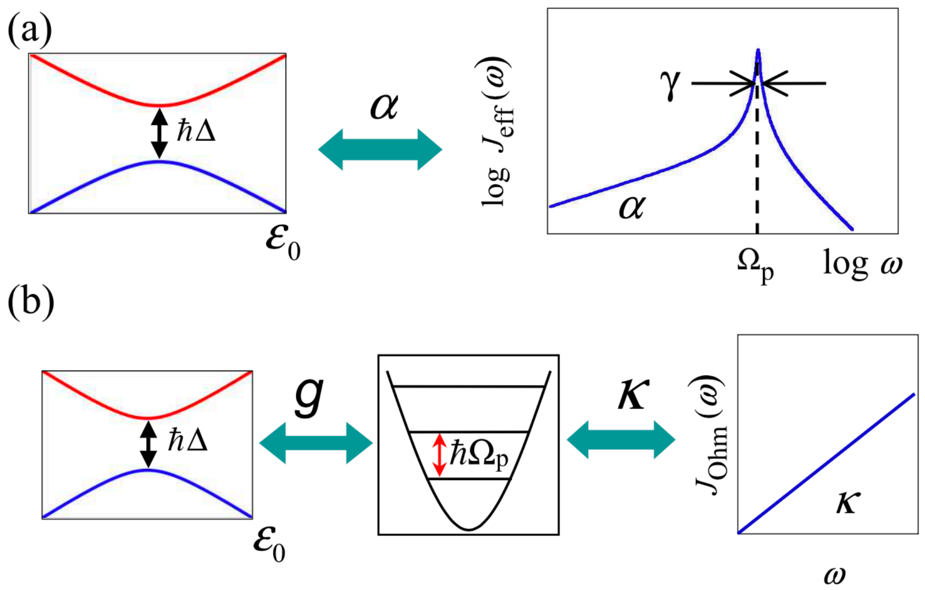
$$J(\omega) = \frac{2\alpha\omega\Omega^4}{(\Omega^2-\omega^2)^2 + (2\pi\kappa\omega\Omega)^2} \stackrel{\omega\to 0}{\longrightarrow} 2\alpha\omega.$$



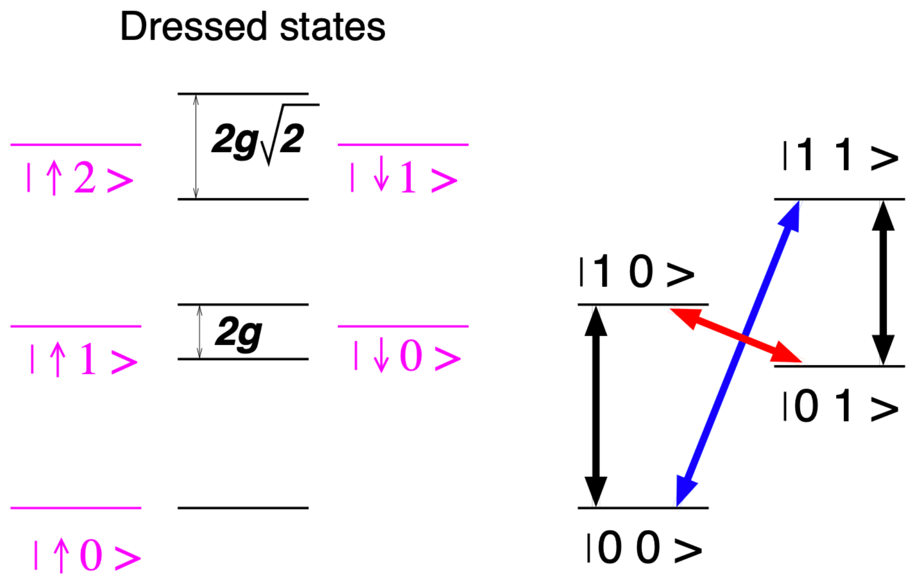
M. Thorwart, E. Paladino, M. Grifoni, Chem. Phys. **296**, 333 (2004)

Superconducting qubit + readout

Garg, Onuchic, Ambegaokar, J. Chem. Phys. **83**, 4491 (1985)



$$g = \sqrt{\pi\alpha\Omega_p^3/4\gamma}, \qquad \kappa = \gamma/2\pi\Omega_p$$



M. Thorwart, E. Paladino, M. Grifoni, Chem. Phys. **296**, 333 (2004)

Superconducting qubit + readout

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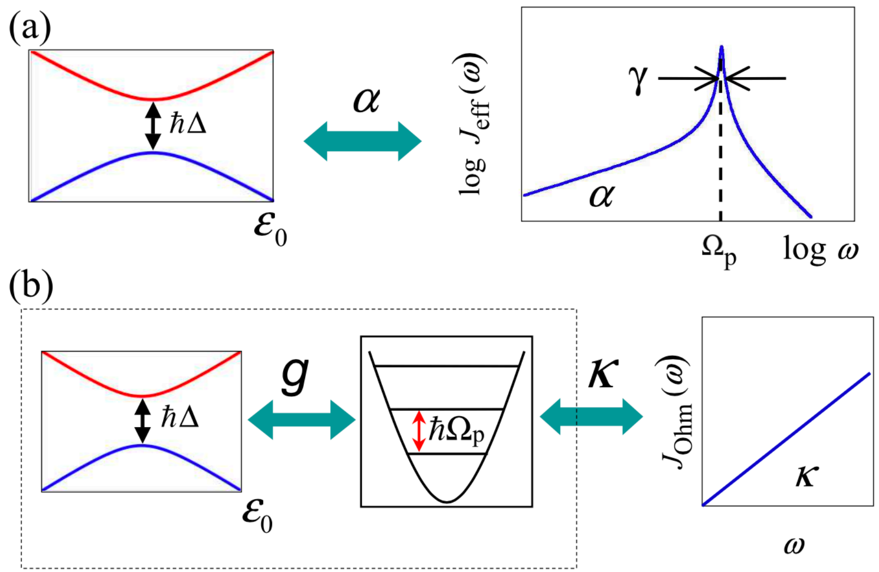
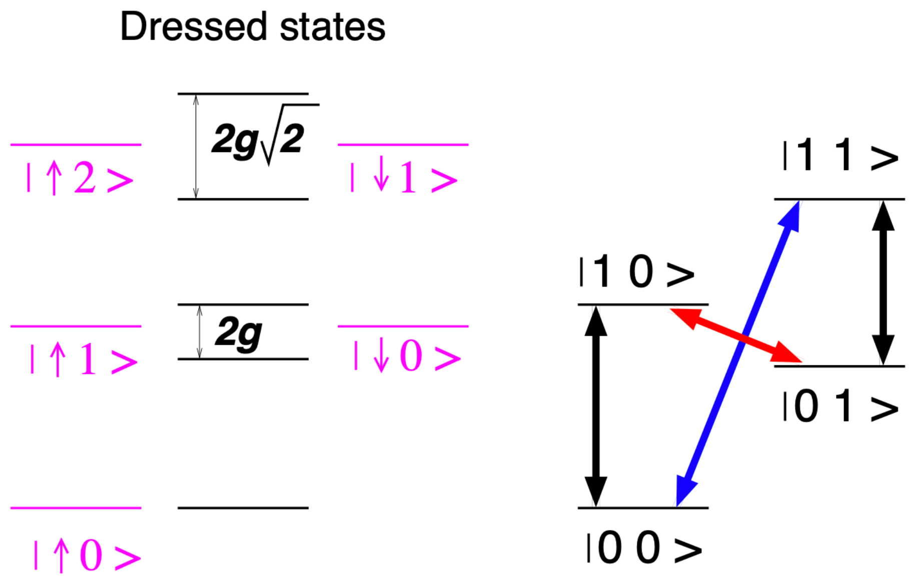


H_S

$$g = \sqrt{\pi\alpha\Omega_p^3/4\gamma}, \qquad \kappa = \gamma/2\pi\Omega_p$$



M. Thorwart, E. Paladino, M. Grifoni, Chem. Phys. **296**, 333 (2004)

Superconducting qubit + readout

Compute symmetrized qubit autocorrelation function:

$$S_z(t) = \frac{1}{2}\langle \sigma_z(t)\sigma_z(0) + \sigma_z(0)\sigma_z(t)\rangle - \langle \sigma_z \rangle^2_{\infty,+}$$

and its half-sided Fourier transform $S_z(\omega) = 2\int_0^\infty \mathrm{d}t \cos\omega t\, S_z(t)$

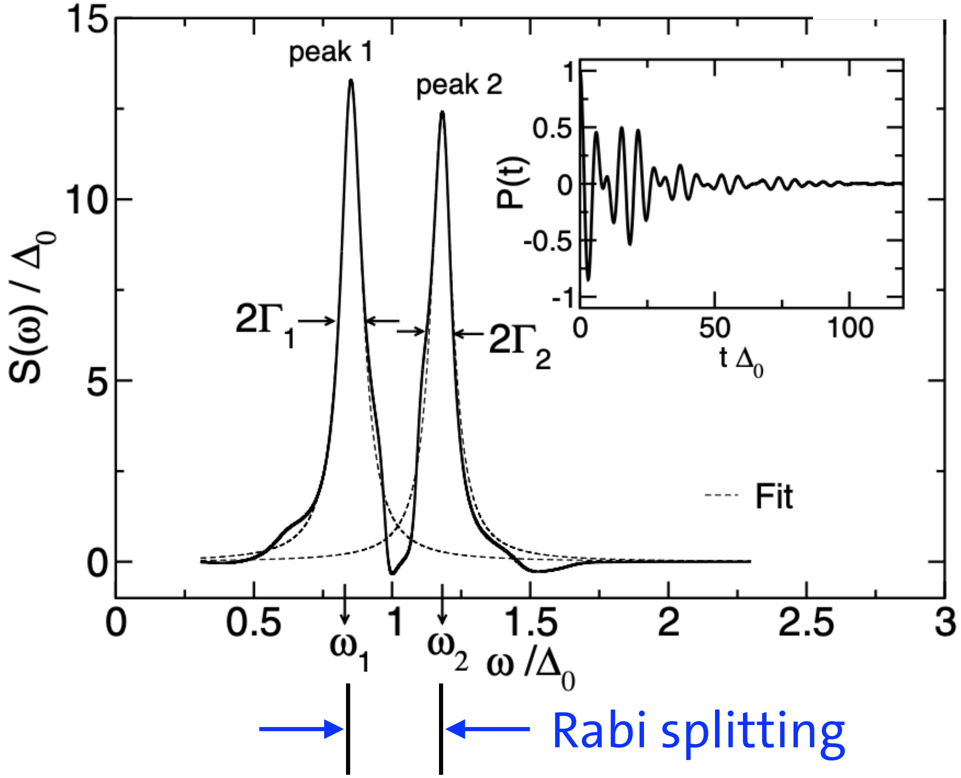
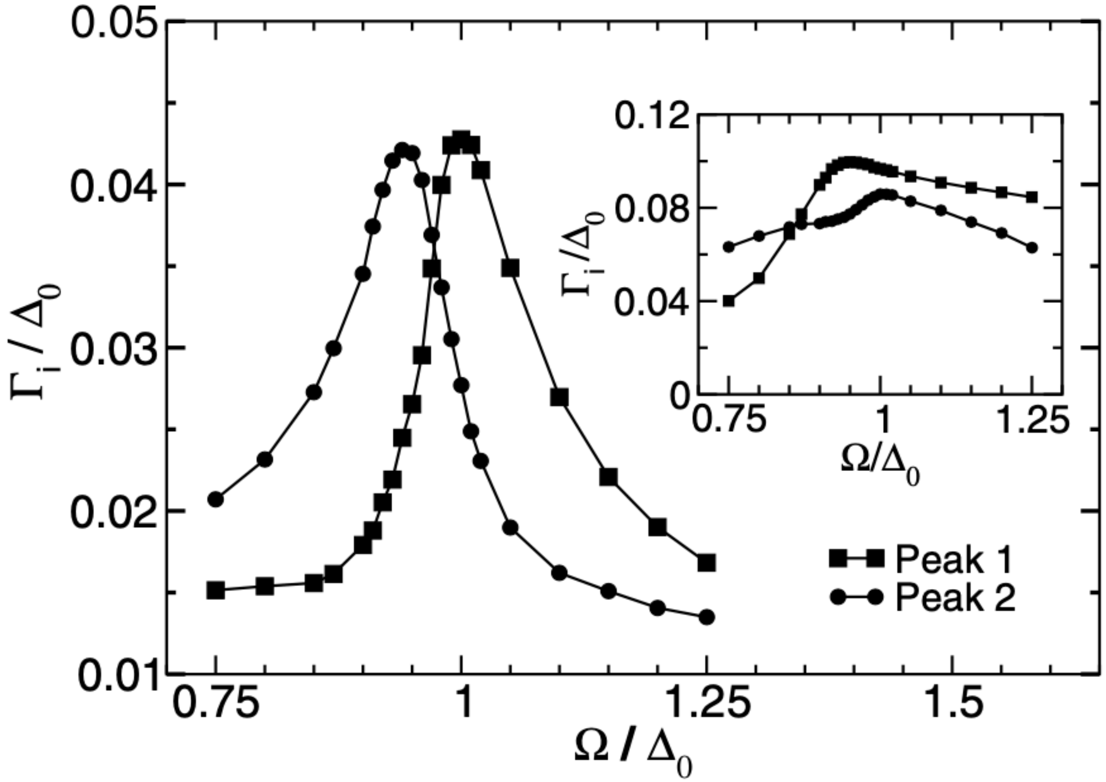


Fig. 1. Example of the dynamics for the symmetric case $\varepsilon = 0$, where the oscillator frequency is in resonance with the TSS frequency, i.e., $\Omega = \Delta_0$. Parameters are: $g = 0.18\Delta_0$, $\kappa = 0.014$ $(\to \alpha = 0.004)$, $k_B T = 0.1\hbar\Delta_0$. QUAPI parameters are $M = 12$, $K = 1$, $\Delta t = 0.06/\Delta_0$.

M. Thorwart, E. Paladino, M. Grifoni, Chem. Phys. **296**, 333 (2004)

Superconducting qubit + readout

symmetric qubit: dephasing rates



Simple one-phonon rate with peaked bath

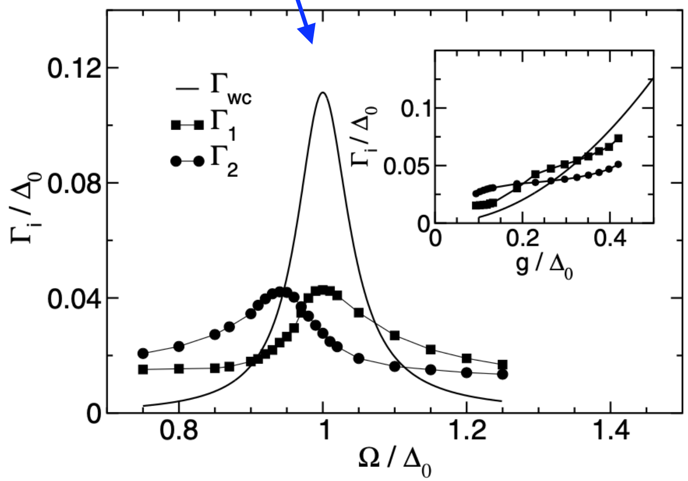


Fig. 9. Dephasing rates Γ_1 and Γ_2 in comparison with the weak-coupling rate Γ_d for varying Ω. Parameters are: $\varepsilon = 0$, $g = 0.07\Delta_0$, $\kappa = 0.014$ ($\rightarrow \alpha = 0.0005$ for $\Omega = \Delta_0$), $k_B T = 0.1\hbar\Delta_0$. Inset: Corresponding results for varying g for $\Omega = 0.75\Delta_0$.

M. Thorwart, E. Paladino, M. Grifoni, Chem. Phys. **296**, 333 (2004)

Qubit in a sub-Ohmic heat bath

$$\hat{H} = \hat{H}_S + \hat{H}_{\rm env} = \hat{H}_S + \sum_j \left[\frac{\hat{p}_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 \left(\hat{x}_j - \frac{c_j \hat{s}}{m_j \omega_j^2} \right)^2 \right]$$

$$\rho_{\rm env}(0) \propto e^{-\hat{H}_{\rm env}/(k_B T)}$$

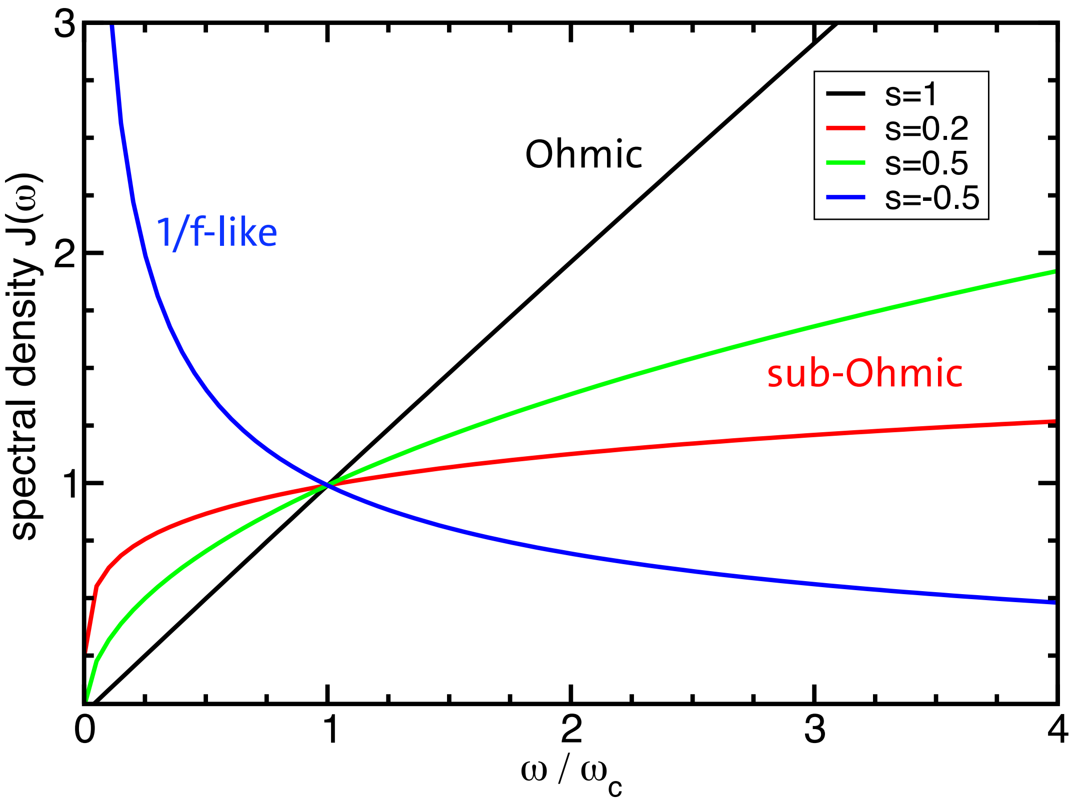
$$\rho_S(0) = |\uparrow\rangle$$

$$\omega_c = 10\Omega\,, \quad T = 0$$

$$\hat{H}_S = \frac{\Omega}{2}\hat{\sigma}_x \qquad \hat{s} = \frac{1}{2}\hat{\sigma}_z$$

spectral exponent $0 \leq s \leq 1$

$$J(\omega) = 2\alpha \frac{\omega^s}{\omega_c^{s-1}} \exp\left(-\frac{\omega}{\omega_c}\right)$$

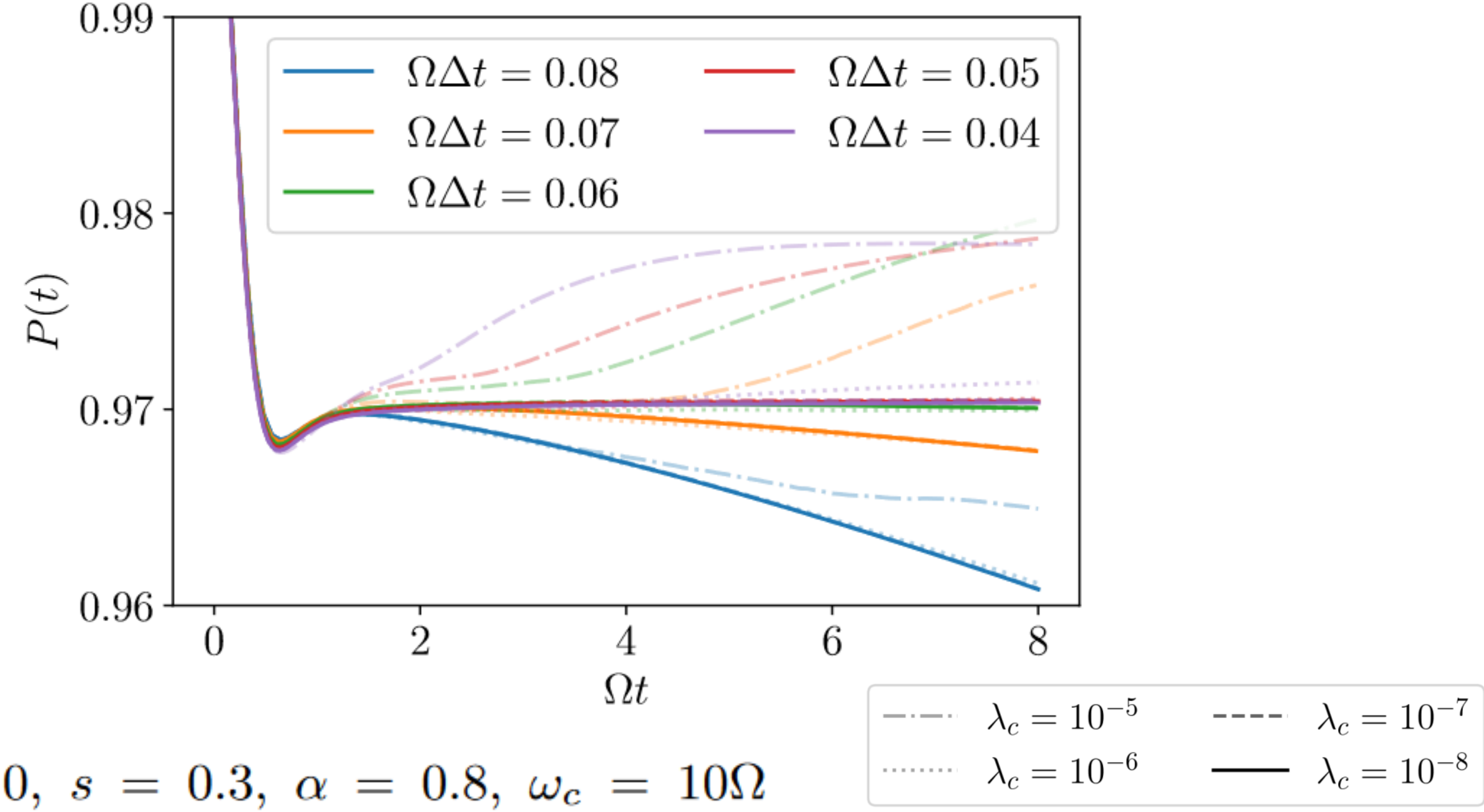


F. Otterpohl, P. Nalbach, M. Thorwart, Phys. Rev. Lett. **129**, 120406 (2022)

Qubit in a sub-Ohmic heat bath

Compute polarization: $P(t) := \langle \hat{\sigma}_z \rangle_t$

Two (controlled) approximations: discrete time step Δt and singular value cutoff λ_c

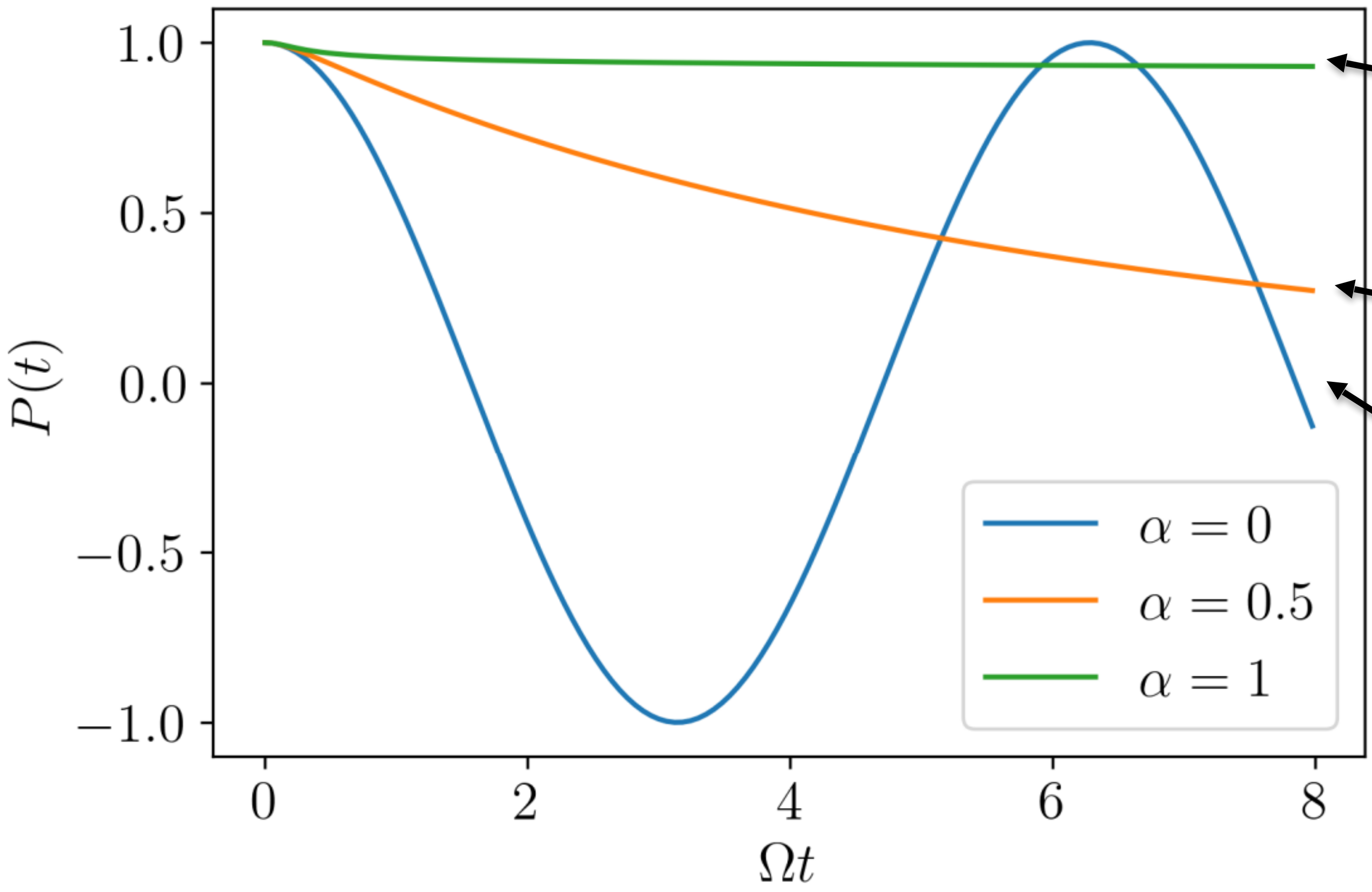


$T = 0, \; s = 0.3, \; \alpha = 0.8, \; \omega_c = 10\Omega$

F. Otterpohl, P. Nalbach, M. Thorwart, Phys. Rev. Lett. **129**, 120406 (2022)

Qubit in a sub-Ohmic heat bath

Typical behavior, Ohmic bath:



$$P(t) \xrightarrow[\omega_c \to \infty]{} 1$$

$$P(t) \xrightarrow[\omega_c \to \infty]{} \exp\left(-\frac{\pi}{2}\frac{\Omega^2}{\omega_c}t\right)$$

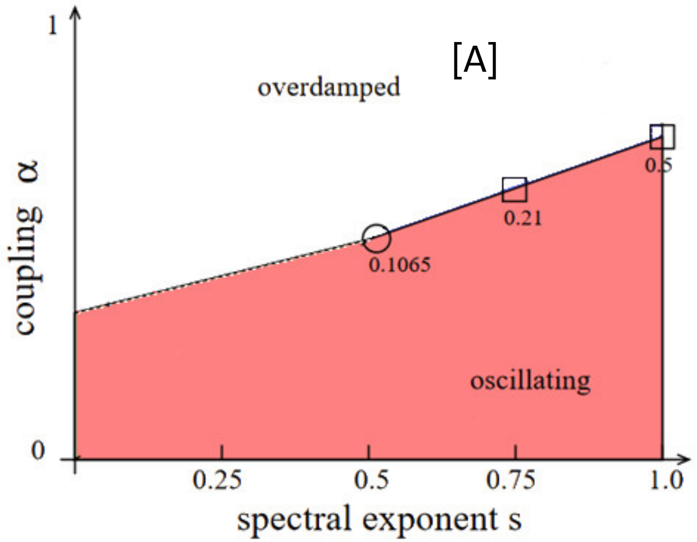
$$P(t) = \cos(\Omega t)$$

F. Otterpohl, P. Nalbach, M. Thorwart, Phys. Rev. Lett. **129**, 120406 (2022)

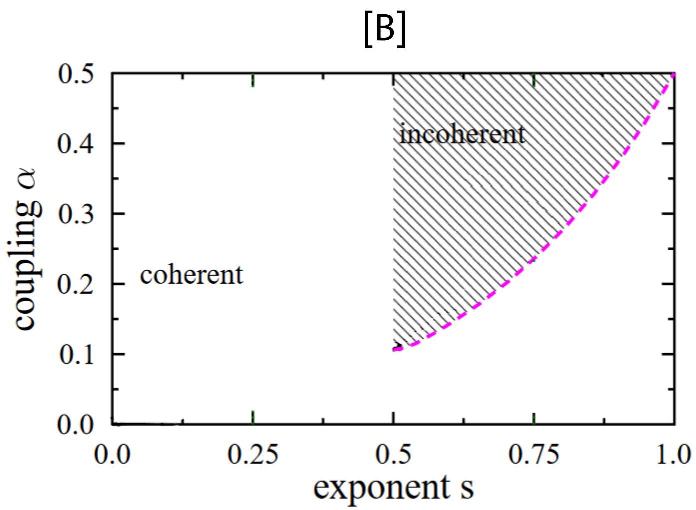
Qubit in a sub-Ohmic heat bath

$\omega_c = 10\Omega,\, T = 0$

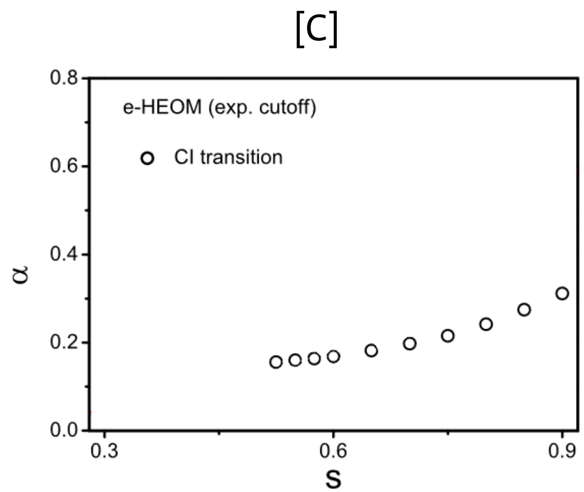
Literature on dynamical phase diagram for $s \leq 1$



QUAPI



PI Monte Carlo



HEOM

all plots are adapted to contain only information about coherent-incoherent transition

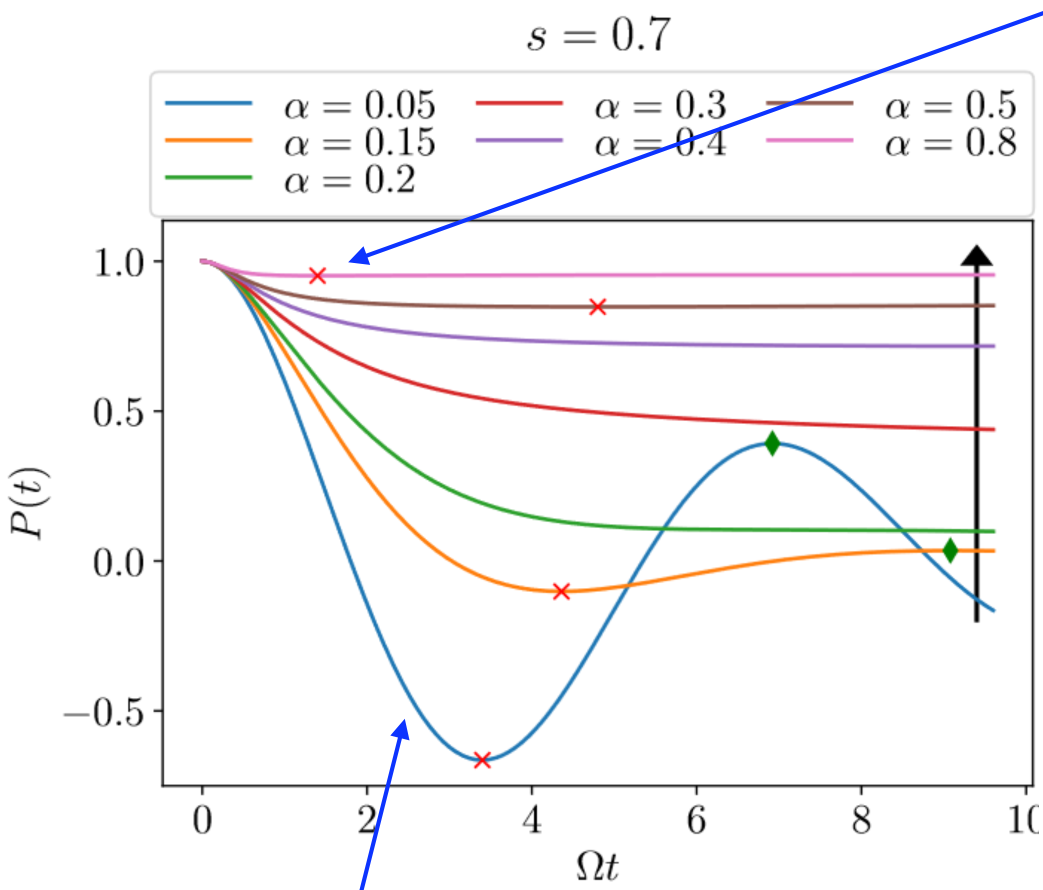
[A] P. Nalbach, M. Thorwart, *Ultraslow Quantum Dynamics in a Sub-Ohmic Heat Bath*, Phys. Rev. B **81**, 054308 (2010)

[B] D. Kast, J. Ankerhold, *Persistence of Coherent Quantum Dynamics at Strong Dissipation*, Phys. Rev. Lett. **110**, 010402 (2013)

[C] C. Duan, Z. Tang, J. Cao, and J. Wu, *Zero-Temperature Localization in a Sub-Ohmic Spin-Boson Model Investigated by an Extended Hierarchy Equation of Motion*, Phys. Rev. B **95**, 214308 (2017)

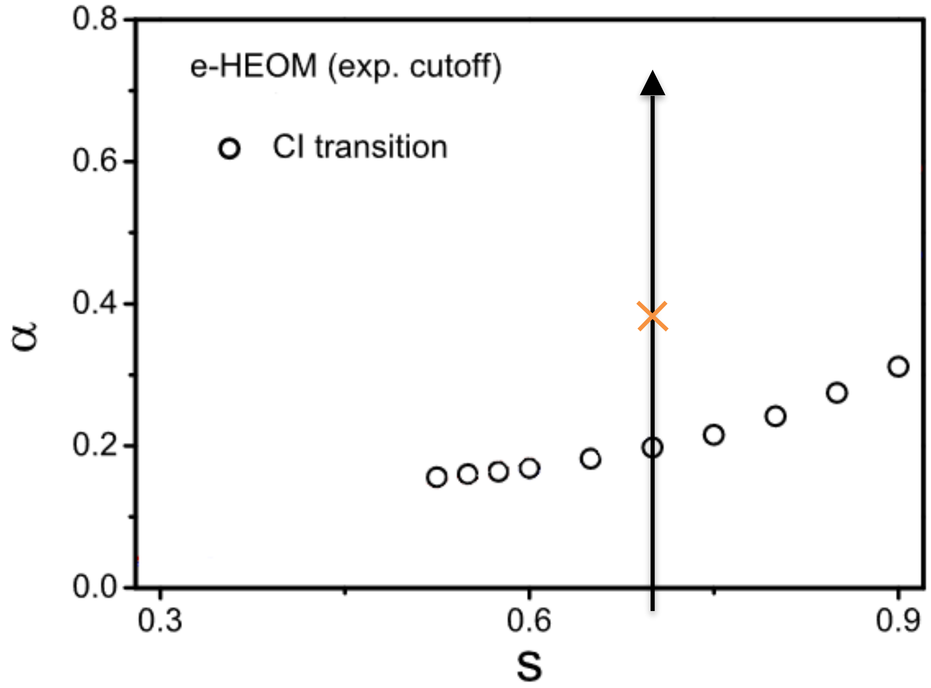
Qubit in a sub-Ohmic heat bath

The case $s = 0.7$



Still minimum at very strong damping ⇒ coherence?

[C]



„Ordinary“ coherent oscillations at weak coupling

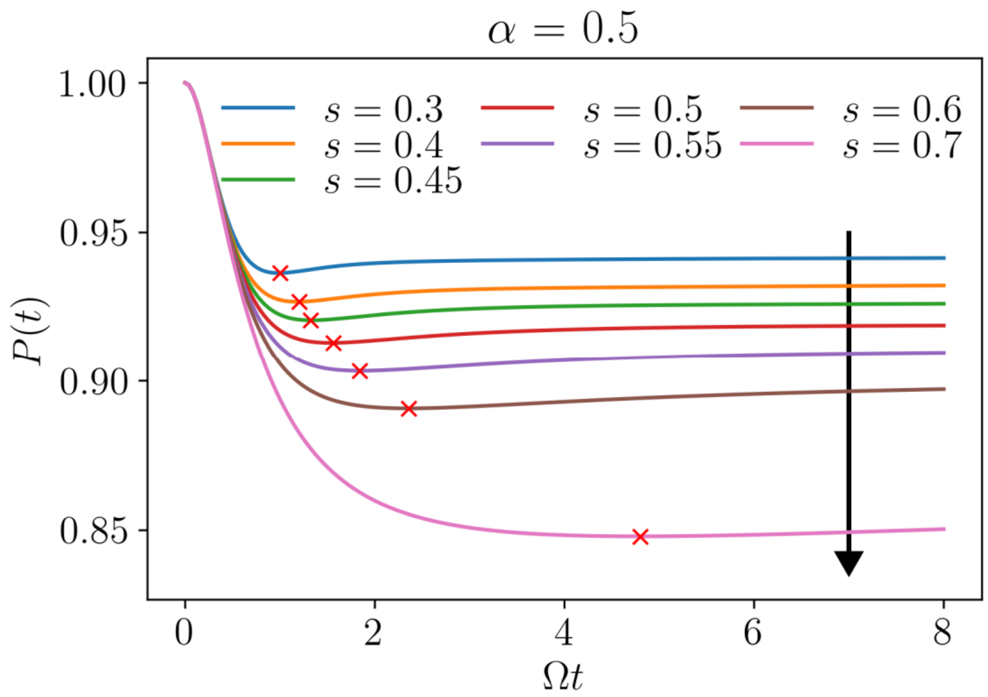
[C] C. Duan, Z. Tang, J. Cao, J. Wu, Phys. Rev. B **95**, 214308 (2017)

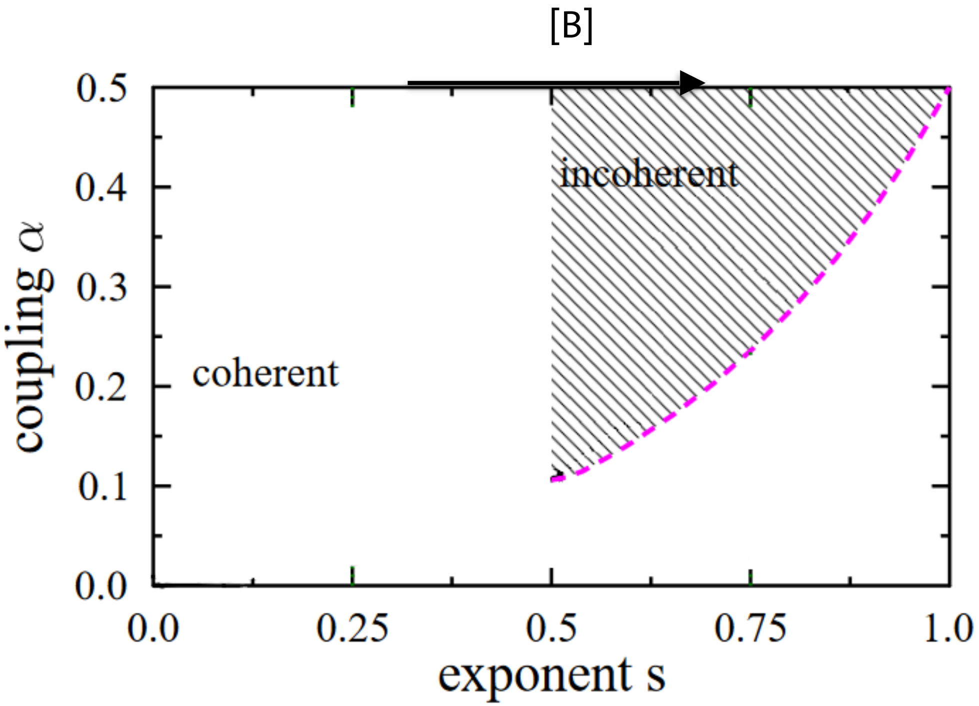
Such a remaining coherence is not found in [C]

F. Otterpohl, P. Nalbach, M. Thorwart, Phys. Rev. Lett. **129**, 120406 (2022)

Qubit in a sub-Ohmic heat bath

Coherent-incoherent transition at $s = 0.5$?





Minimum coherence always remains when tuning s

[B] D. Kast and J. Ankerhold, Phys. Rev. Lett. **110**, 010402 (2013)

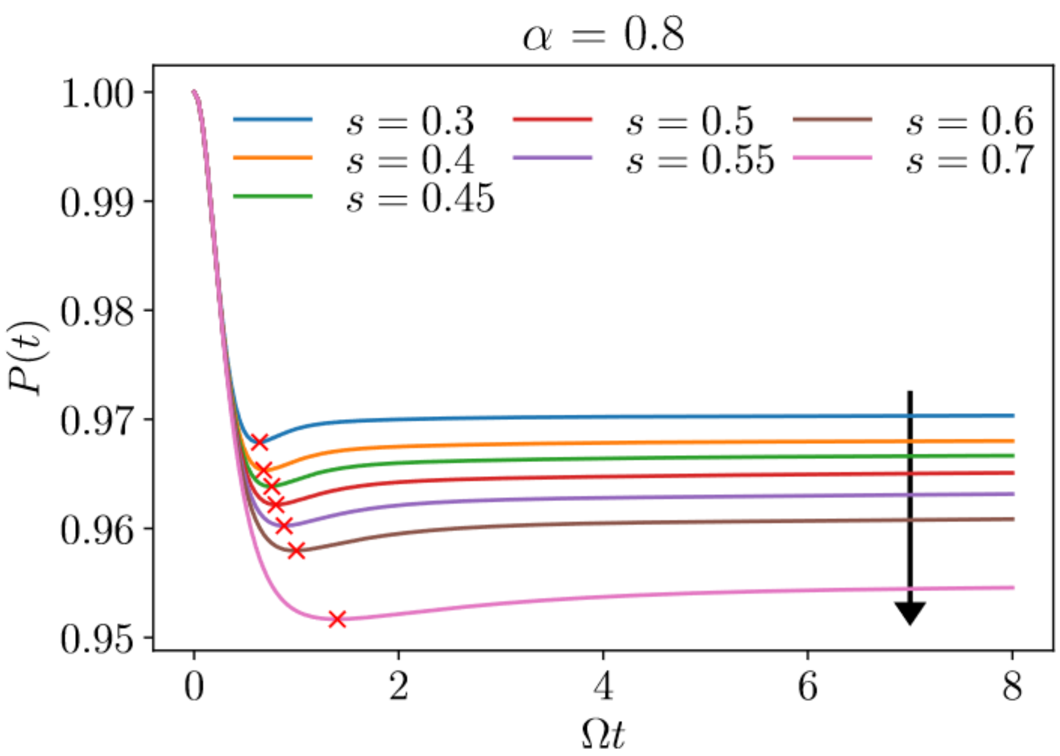
This transition is not recovered by us

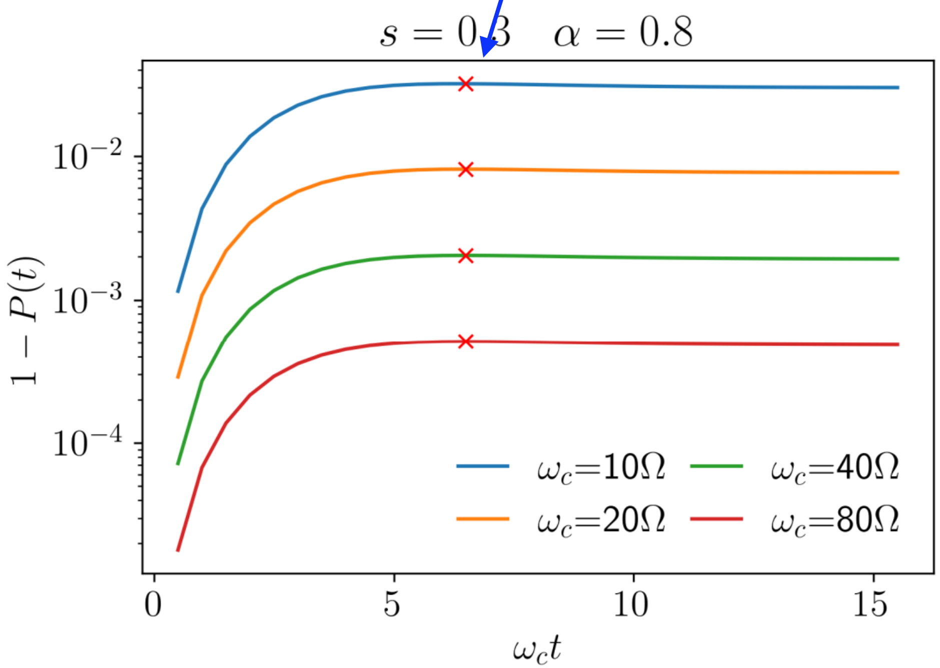
F. Otterpohl, P. Nalbach, M. Thorwart, Phys. Rev. Lett. **129**, 120406 (2022)

Qubit in a sub-Ohmic heat bath

Pseudo-coherent phase:
Bath dominates dynamics at strong coupling

Minimum determined by $\propto \omega_c^{-1}$



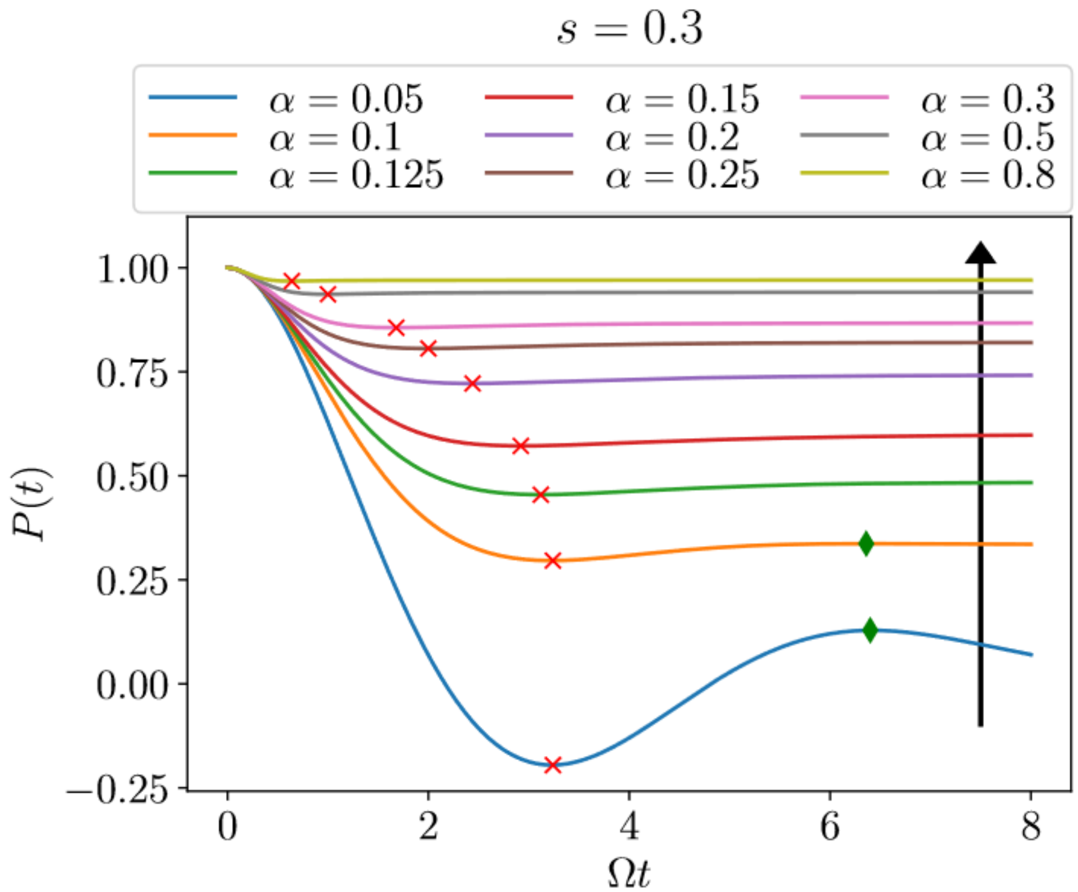


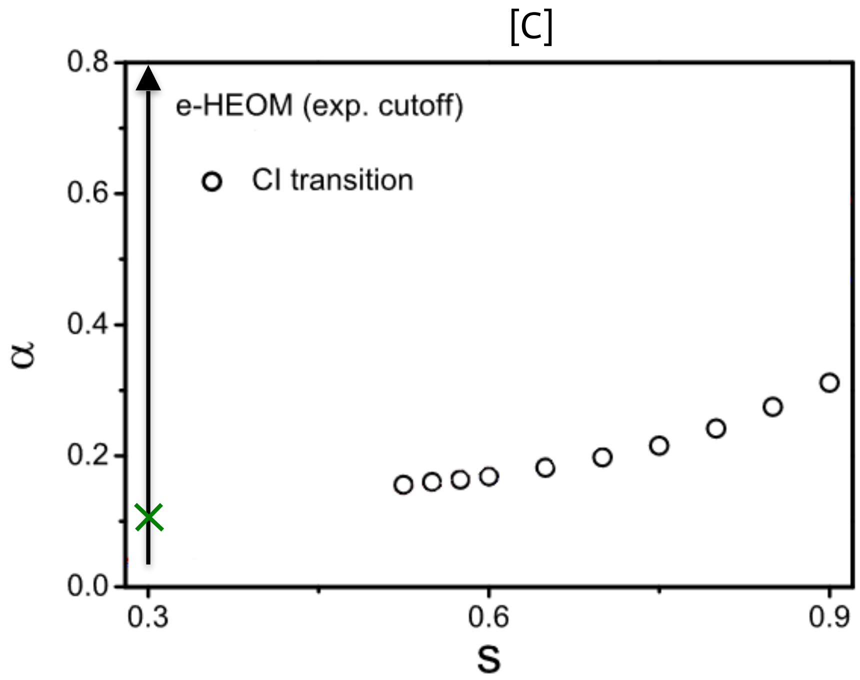
Minimum coherence always remains when tuning s

F. Otterpohl, P. Nalbach, M. Thorwart, Phys. Rev. Lett. **129**, 120406 (2022)

Qubit in a sub-Ohmic heat bath

Coherent to Pseudo-coherent phase transition at small s



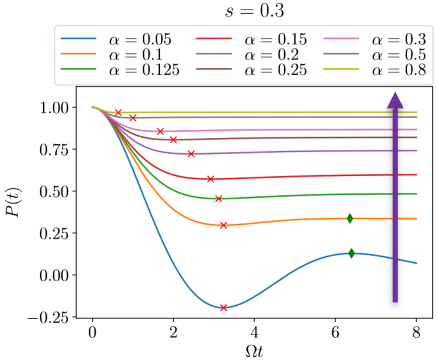


[C] C. Duan, Z. Tang, J. Cao, and J. Wu, Phys. Rev. B **95**, 214308 (2017)

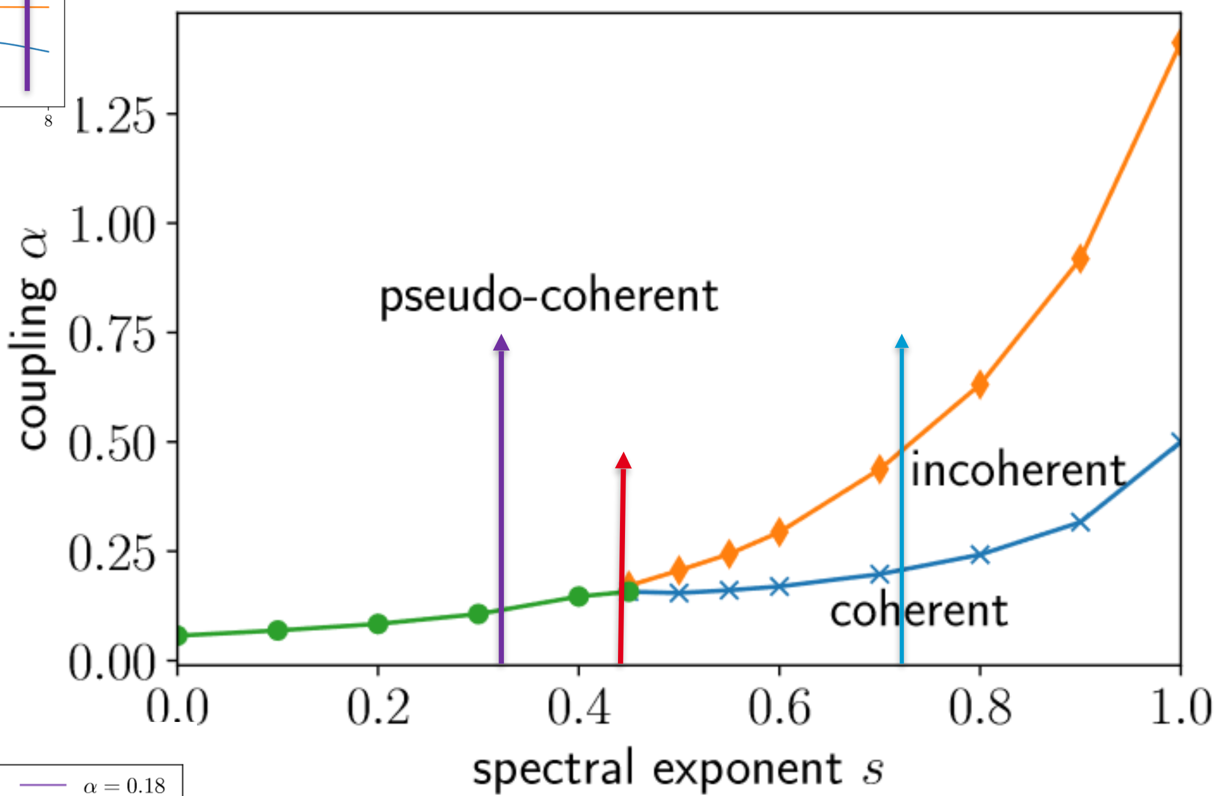
F. Otterpohl, P. Nalbach, M. Thorwart, Phys. Rev. Lett. **129**, 120406 (2022)

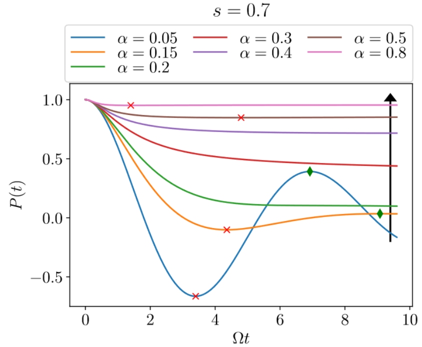
Qubit in a sub-Ohmic heat bath

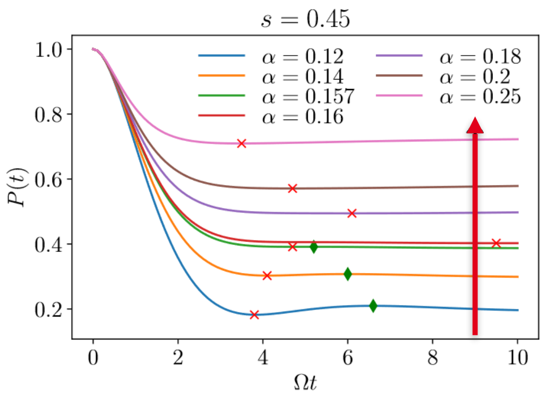
$T = 0,\ \omega_c = 10\Omega$



The Phase Diagram







F. Otterpohl, P. Nalbach, M. Thorwart, Phys. Rev. Lett. **129**, 120406 (2022)

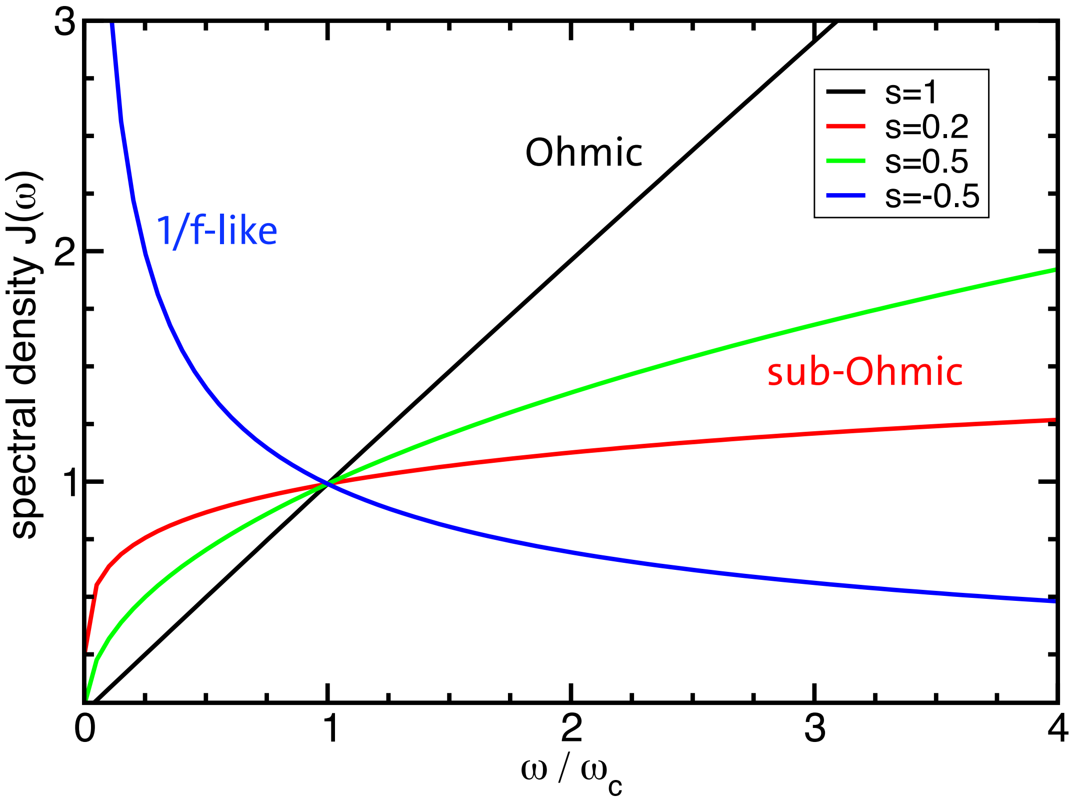
Qubit exposed to quantum 1/f noise

$$\hat{H} = \hat{H}_S + \hat{H}_{\rm env} = \hat{H}_S + \sum_j \left[\frac{\hat{p}_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 \left(\hat{x}_j - \frac{c_j \hat{s}}{m_j \omega_j^2} \right)^2 \right]$$

$$\rho_{\rm env}(0) \propto e^{-\hat{H}_{\rm env}/(k_B T)}$$

$$\rho_S(0) = |\uparrow\rangle$$

$$\hat{H}_S = \frac{\Omega}{2} \hat{\sigma}_x \qquad \hat{s} = \frac{1}{2} \hat{\sigma}_z$$



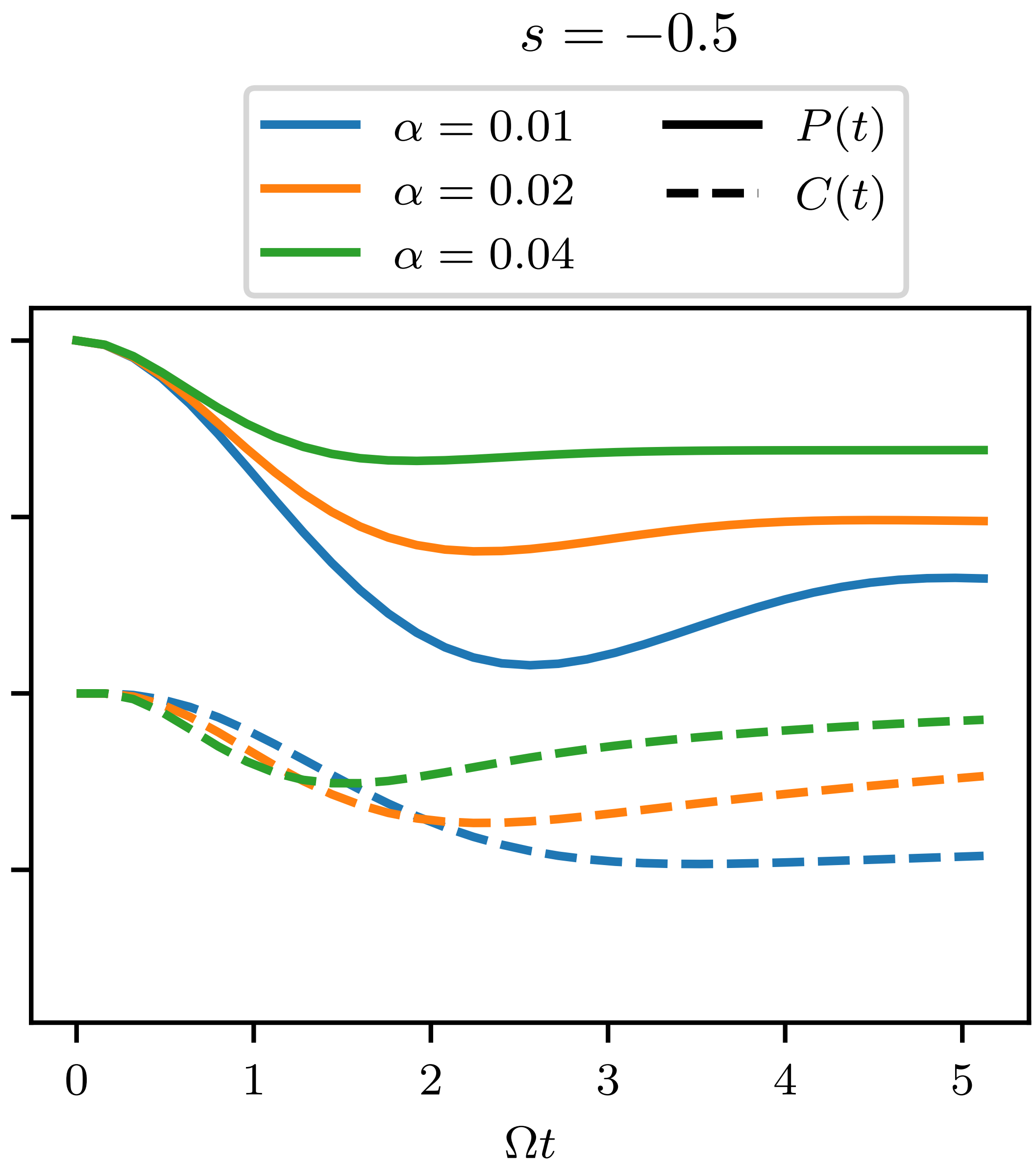
spectral exponent $-1 \leq s \leq 1$

$$J(\omega) = 2\alpha \frac{\omega^s}{\omega_c^{s-1}} e^{-\frac{\omega}{\omega_c}} \Theta(\omega - \omega_{\rm ir})$$

ultraviolet and infrared bath cutoff frequencies

F. Otterpohl, P. Nalbach, E. Paladino, G.A. Falci, M. Thorwart, in review (2025)

Qubit exposed to quantum 1/f noise



Polarization $P(t) = \langle \hat{\sigma}_z \rangle_t$

Coherence $C(t) = \langle \hat{\sigma}_x \rangle_t$

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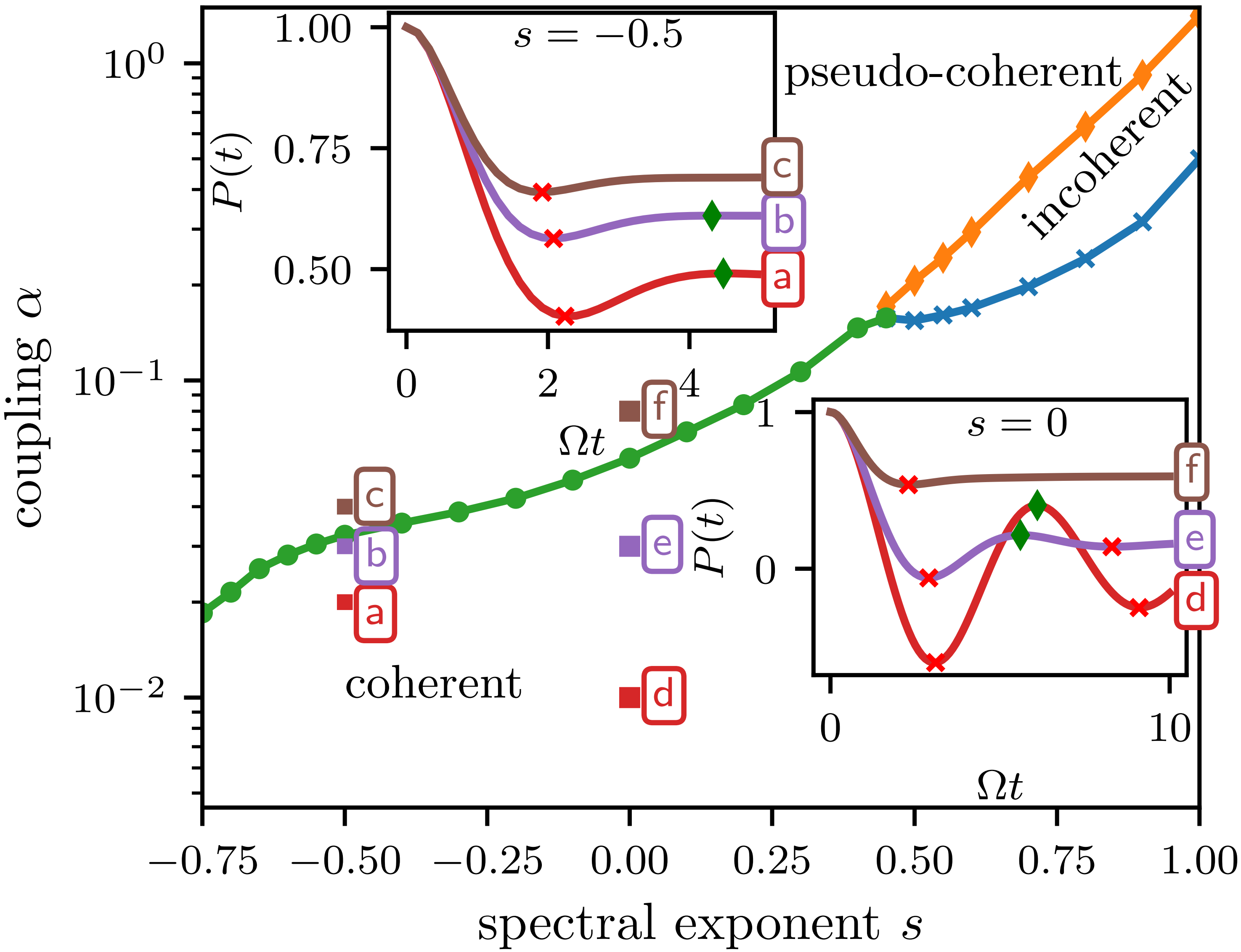
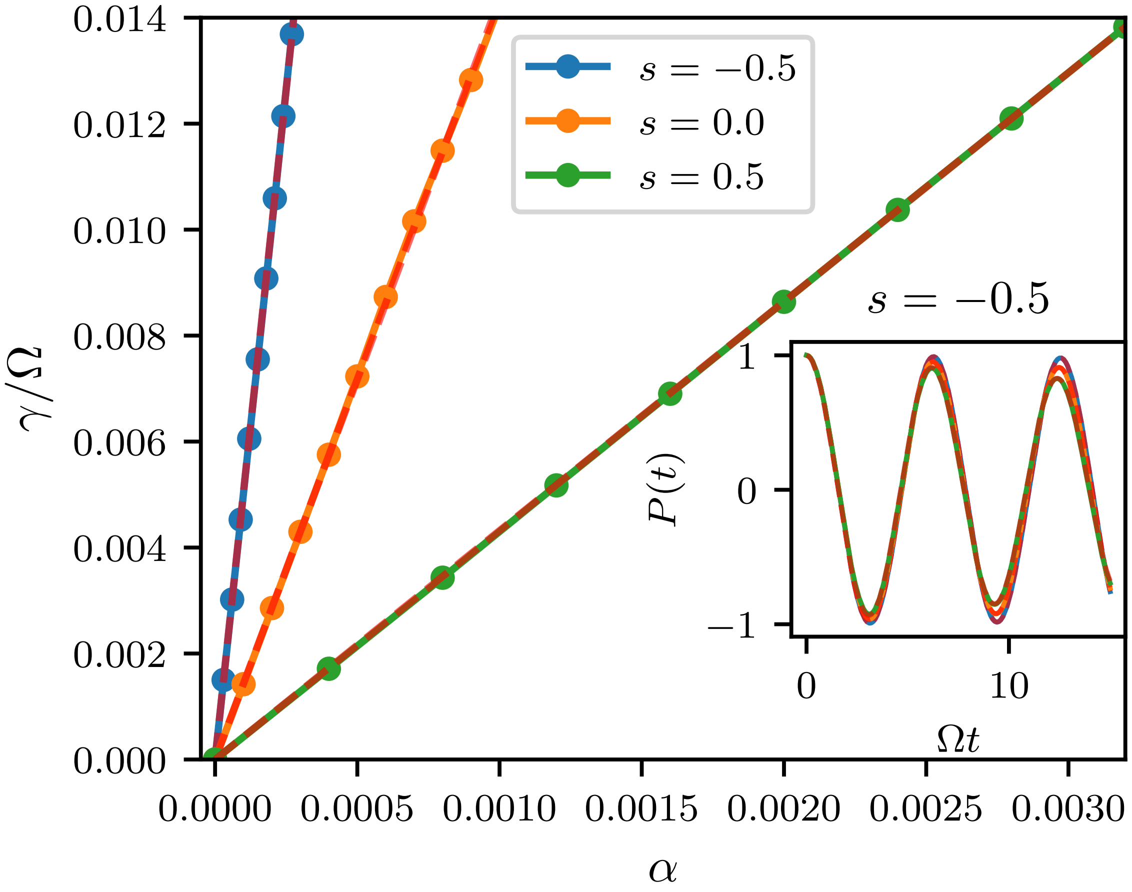
Qubit exposed to quantum 1/f noise

The Phase Diagram



F. Otterpohl, P. Nalbach, E. Paladino, G.A. Falci, M. Thorwart, in review (2025)

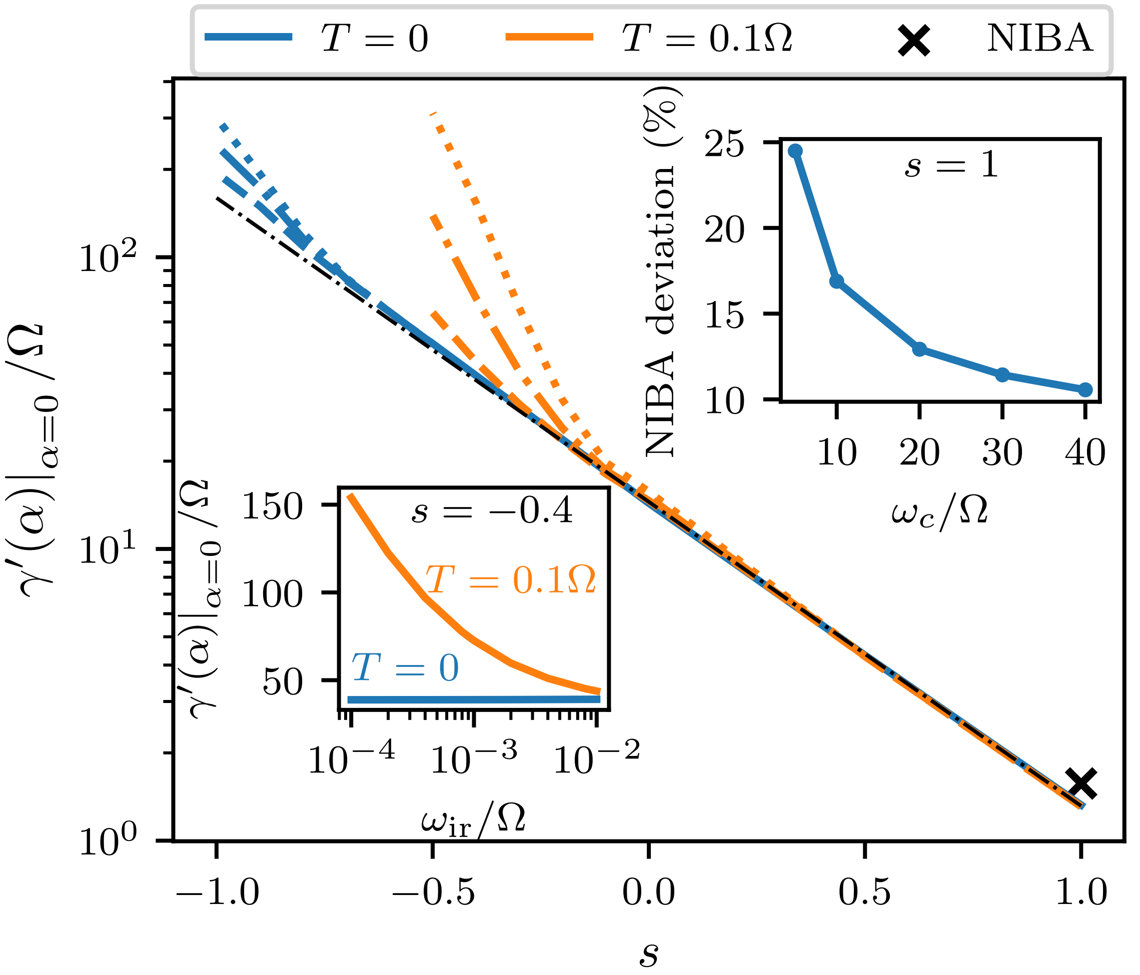
Qubit exposed to quantum 1/f noise



Linear dependence of dephasing rate on damping strength

F. Otterpohl, P. Nalbach, E. Paladino, G.A. Falci, M. Thorwart, in review (2025)

Qubit exposed to quantum 1/f noise

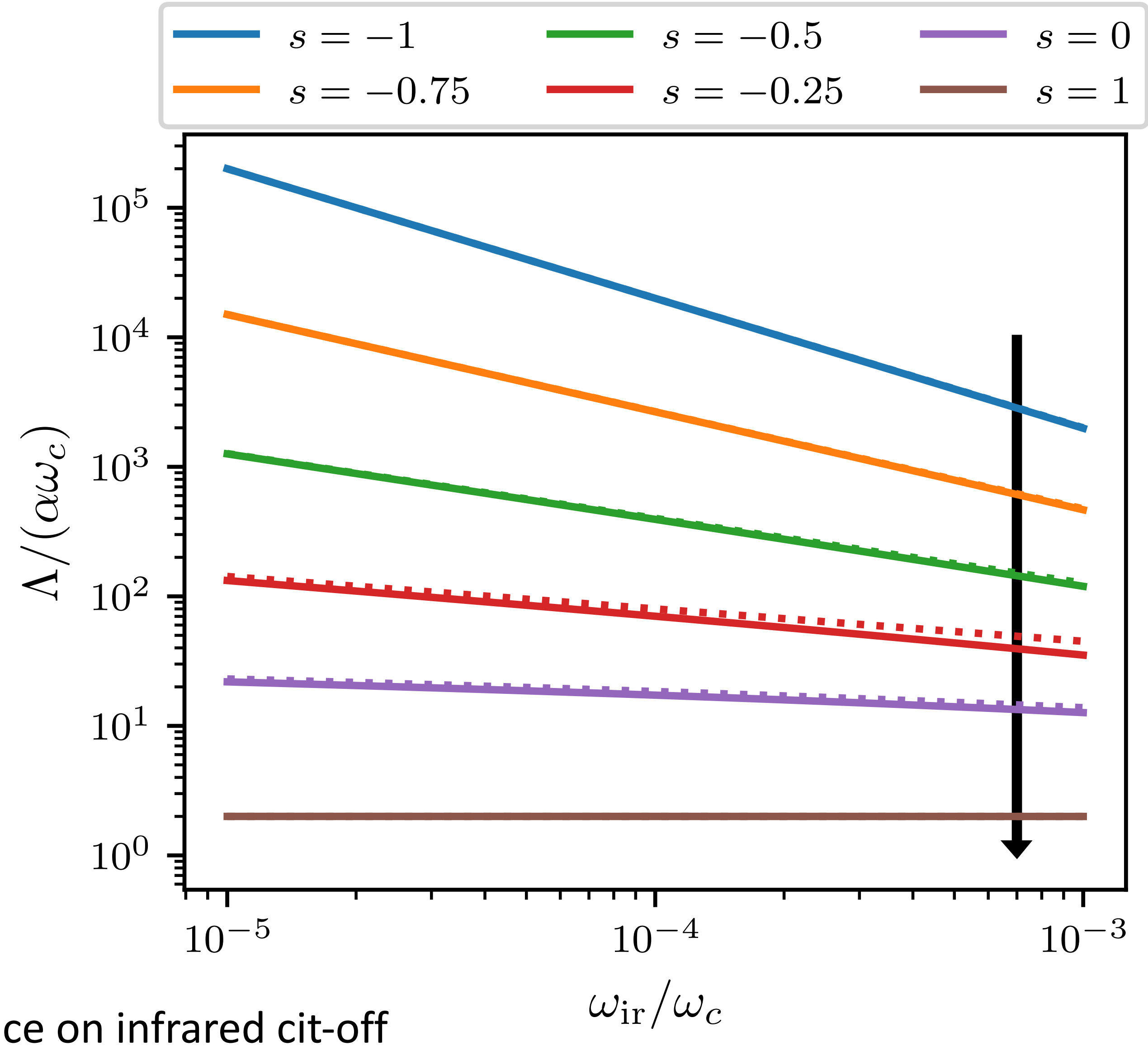


Role of finite temperature

Relation to NIBA lowest order rate

F. Otterpohl, P. Nalbach, E. Paladino, G.A. Falci, M. Thorwart, in review (2025)

Qubit exposed to quantum 1/f noise



Dependence on infrared cit-off

F. Otterpohl, P. Nalbach, E. Paladino, G.A. Falci, M. Thorwart, in review (2025)

Qubit exposed to quantum 1/f noise

Note:

- In many cases, ultraslow relaxation and strong coupling to low-frequency bath modes are known to occur
- Physical origin: quantum two-level fluctuators in the environment (amorphous solids)
- Such types of fluctuations are clearly non-Gaussian and are not captured by a spin-boson model with s>0

Decoherence and 1/*f* Noise in Josephson Qubits

E. Paladino,[1] L. Faoro,[2] G. Falci,[1] and Rosario Fazio[3]

Phys. Rev. Lett. **88**, 228304 (2002)

REVIEWS OF MODERN PHYSICS, VOLUME 86, APRIL–JUNE 2014

1/*f* noise: Implications for solid-state quantum information

E. Paladino*, Y. M. Galperin†, G. Falci‡, and B. L. Altshuler§

Rev. Mod. Phys. **86**, 361 (2014)

F. Otterpohl, P. Nalbach, E. Paladino, G.A. Falci, M. Thorwart, in review (2025)

Superconducting qubit in non-commuting baths

$$\hat{H} = \hat{H}_{\mathrm{S}} + \hat{H}_{\mathrm{env},\,1} + \hat{H}_{\mathrm{env},\,2} = \hat{H}_{\mathrm{S}} + \sum_j \left[\frac{\hat{p}_{1,j}^2}{2m_{1,j}} + \frac{1}{2} m_{1,j} \omega_j^2 \left(\hat{x}_{1,j} - \frac{c_{1,j}\hat{s}_1}{m_{1,j}\omega_{1,j}^2} \right)^2 \right] + \sum_j \left[\frac{\hat{p}_{2,j}^2}{2m_{2,j}} + \frac{1}{2} m_{2,j} \omega_j^2 \left(\hat{x}_{2,j} - \frac{c_{2,j}\hat{s}_2}{m_{2,j}\omega_{2,j}^2} \right)^2 \right]$$

where $[\hat{s}_1, \hat{s}_2] \neq 0$

special case: bath 1 is a pure dephasing bath: $\left[\hat{s}_1, \hat{H}_{\mathrm{S}}\right] = 0$

➡ Two influence functionals: $F_1(\beta_0, \beta_1, ..., \beta_N) = F_1(\beta_0, \beta_1, ..., \beta_N)\left[J_1(\omega)\right]$

$$F_2(\alpha_0, \alpha_1, ..., \alpha_N) = F_2(\alpha_0, \alpha_1, ..., \alpha_N)\left[J_2(\omega)\right]$$

T. Palm, The Two Level System under the Influence of Non-Commuting Fluctuations, PhD thesis, 2020

F. Otterpohl, P. Nalbach, M. Thorwart, in progress (2025)

Superconducting qubit in non-commuting baths

system-propagator,
single bath:

$$G\left(i_{k+1}^{\pm}, i_k^{\pm}\right) = \left\langle s_{i_{k+1}^{+}} \middle| e^{-iH_{\mathrm{S}}\Delta t} \middle| s_{i_k^{+}} \right\rangle \left\langle s_{i_k^{-}} \middle| e^{iH_{\mathrm{S}}\Delta t} \middle| s_{i_{k+1}^{-}} \right\rangle$$

➡ two bath case: include change of basis:

$$K\left(i_{k+1}^{\pm}, i_k^{\pm}, j_k^{\pm}\right) = \left\langle s_{2,i_{k+1}^{+}} \middle| e^{-iH_{\mathrm{S}}\Delta t} \middle| s_{1,j_k^{+}} \right\rangle \left\langle s_{1,j_k^{+}} \middle| s_{2,i_k^{+}} \right\rangle \left\langle s_{2,i_k^{-}} \middle| s_{1,j_k^{-}} \right\rangle \left\langle s_{1,j_k^{-}} \middle| e^{iH_{\mathrm{S}}\Delta t} \middle| s_{2,i_{k+1}^{-}} \right\rangle$$

Notation: $\alpha := i^{\pm} \quad \beta := j^{\pm}$

$$\tilde{\rho}_{\alpha_N}^{(N)} = \sum_{\substack{\alpha_0,\ldots,\alpha_{N-1}=1 \\ \beta_0,\ldots,\beta_{N-1}=1}}^{n^2} K(\alpha_0, \ldots, \alpha_N, \beta_0, \ldots, \beta_{N-1}) \tilde{\rho}_{\alpha_0}^{(0)} F_1(\beta_0, \beta_1, \ldots, \beta_{N-1}) F_2(\alpha_0, \alpha_1, \ldots, \alpha_N)$$

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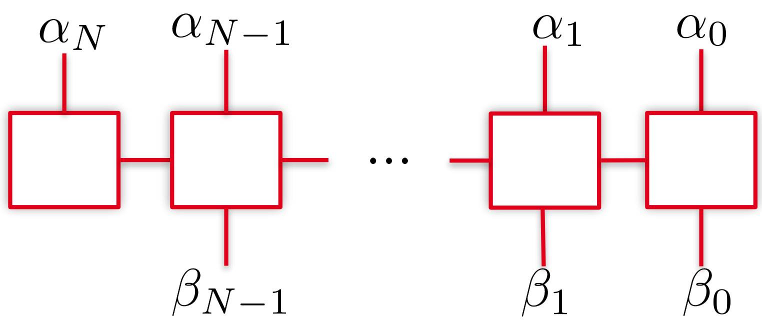
Superconducting qubit in non-commuting baths

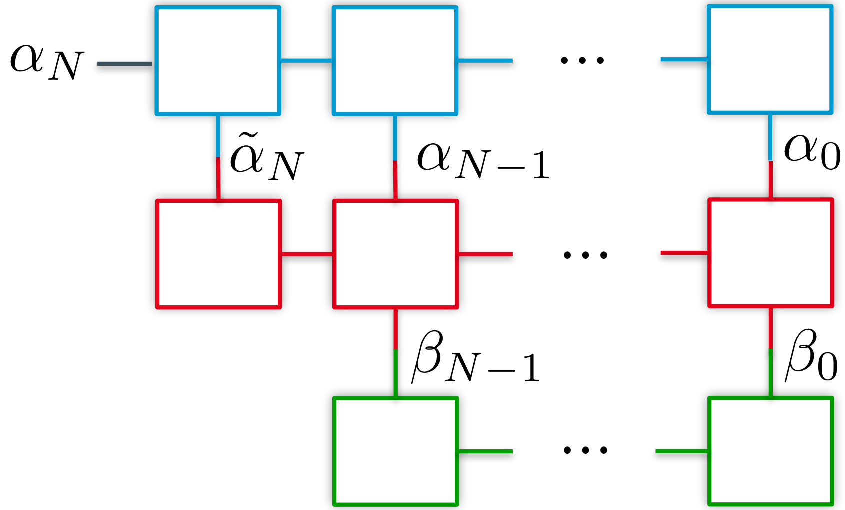
Turn system propagator into MPO:

$$\left(\prod_{k=0}^{N-1} K(\alpha_{k+1}, \alpha_k, \beta_k)\right) = K(\alpha_0, ..., \alpha_N, \beta_0, ..., \beta_{N-1}) =$$



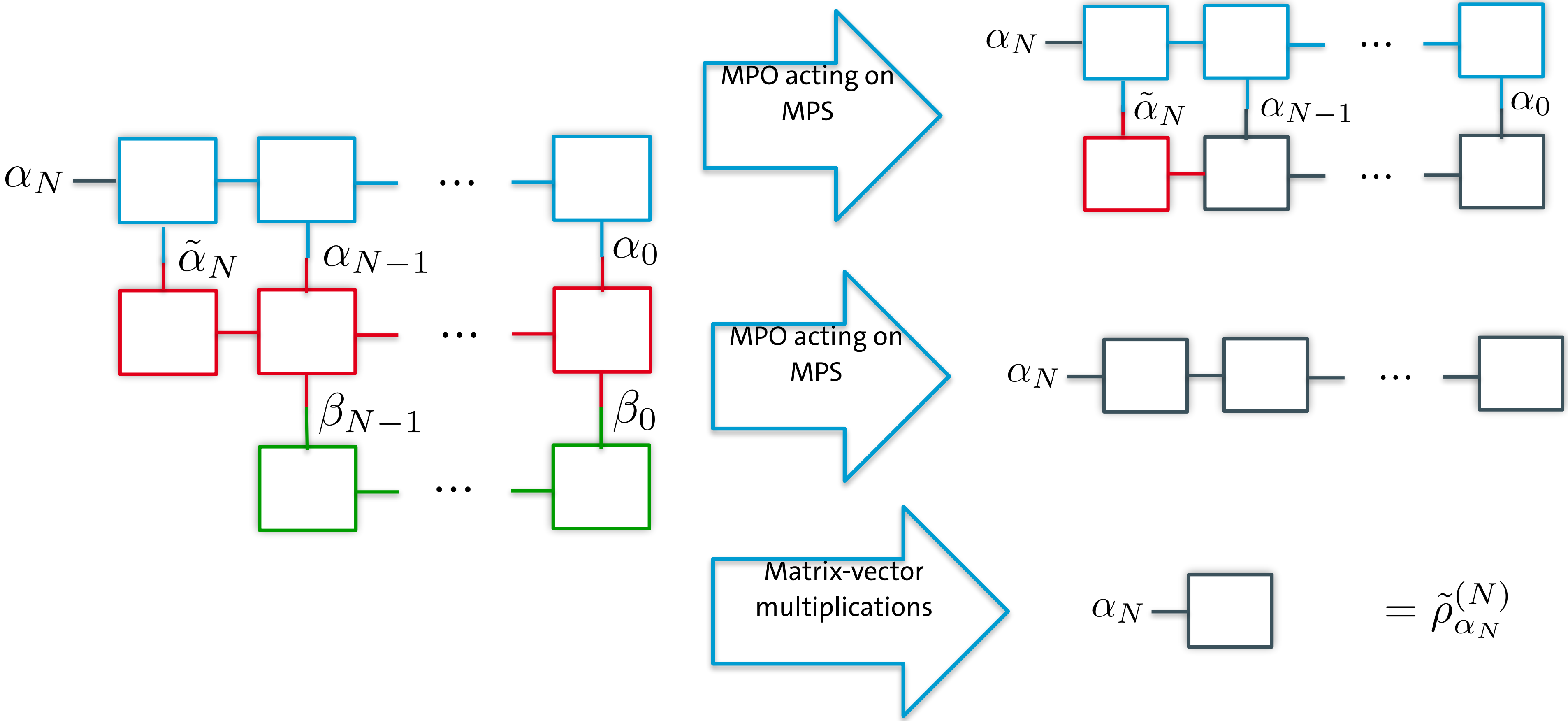
$$\tilde{\rho}_{\alpha_N}^{(N)} = \sum_{\substack{\alpha_0,...,\alpha_{N-1}=1 \\ \beta_0,...,\beta_{N-1}=1}}^{n^2} \underline{K(\alpha_0, ..., \alpha_N, \beta_0, ..., \beta_{N-1})} \tilde{\rho}_{\alpha_0}^{(0)} \underline{F_1(\beta_0, \beta_1, ..., \beta_{N-1})} \underline{F_2(\alpha_0, \alpha_1, ..., \alpha_N)}$$

$$=$$



F. Otterpohl, P. Nalbach, M. Thorwart, in progress (2025)

Superconducting qubit in non-commuting baths



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Superconducting qubit in non-commuting baths

Main finding: disruption of localization transition by a second bath

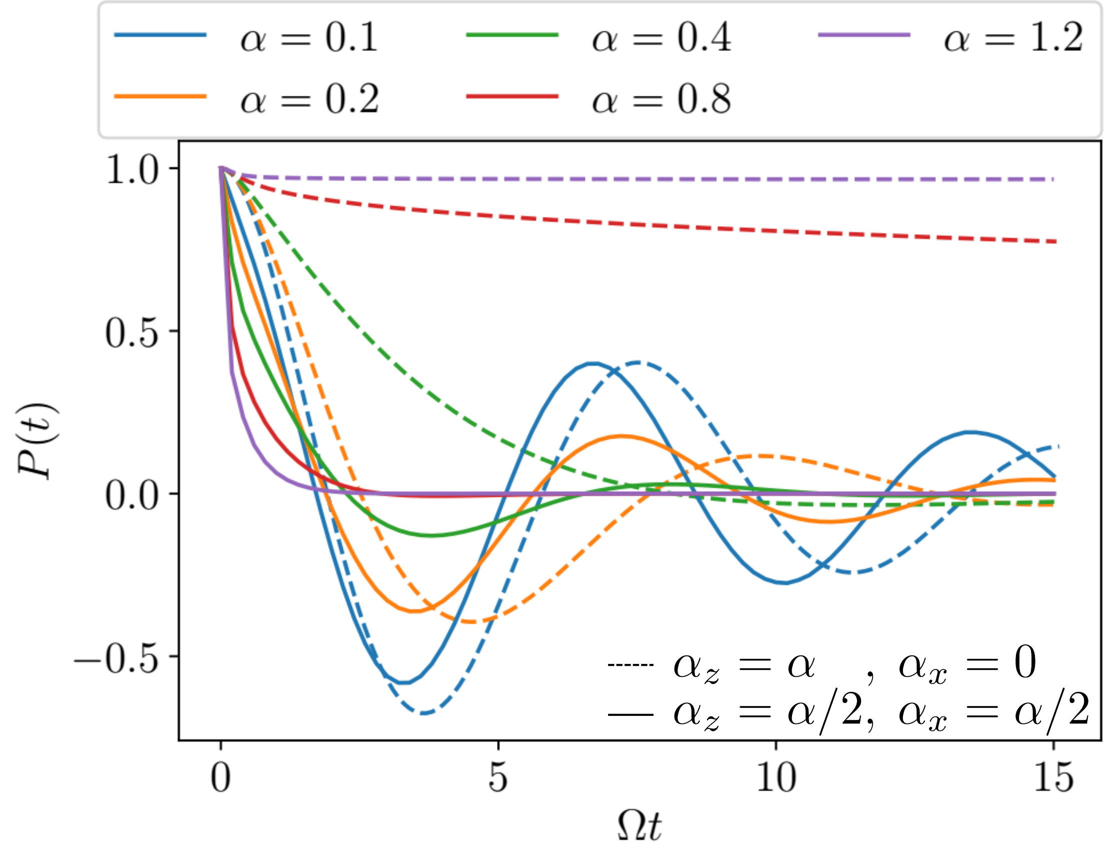
$$J_1(\omega) = 2\alpha_x \omega \exp\left(-\omega/\omega_c\right)$$

$$\hat{s}_1 = \frac{1}{2}\hat{\sigma}_x$$

$$\hat{H}_S = \frac{\Omega}{2}\hat{\sigma}_x$$

$$\hat{s}_2 = \frac{1}{2}\hat{\sigma}_z$$

$$J_2(\omega) = 2\alpha_z \omega \exp\left(-\omega/\omega_c\right)$$



$$\rho_S(0) = |\uparrow\rangle \qquad \rho_{\mathrm{env}}(0) \propto e^{-\hat{H}_{\mathrm{env}}/(k_B T)}$$

$$\omega_c = 10\Omega \quad \text{at } T = 0$$

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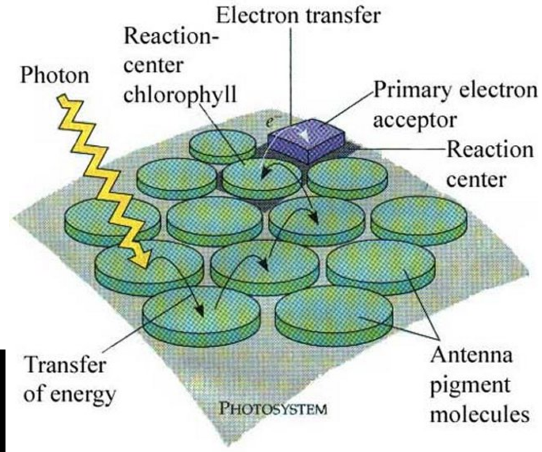
Other techniques (personal selection)

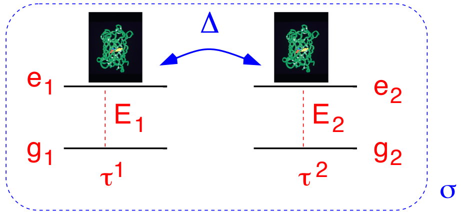
- Quantum Monte Carlo: stochastic sampling of path integral (+: very general, numerically exact, -: sign problem in real time) — Egger, Mak, …
- Stochastic Schrödinger Equation & HOPS (+: very general, very efficient, numerically exact) — Djosi, Strunz, Eisfeld
- Hierarchy Equation of Motion (+: very general, numerically exact) — Tanimura
- Renormalization Groups: DMRG, NRG, fRG, … — Plenio, Burghardt, …
- Flow Equation (+: numerical exact, -: limited to smaller systems) — Kehrein
- Time-Nonlocal Quantum Master Equations (+: very efficient, -: approximative, weak coupling) — Meir, Tannor, …
- Redfield Equation (Born-Markov master equation) (+: very efficient, -: approximative, weak coupling) — Redfield, Bloch, …
- Analytical: NIBA, generalized master equation (+: analytical, -: approximative/perturbative) — Leggett, Weiss, Grabert, Grifoni, Hänggi,…

Examples & applications

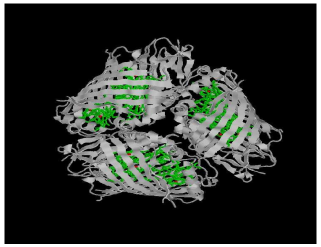
- Quantum transfer of excitation energy / exciton transport



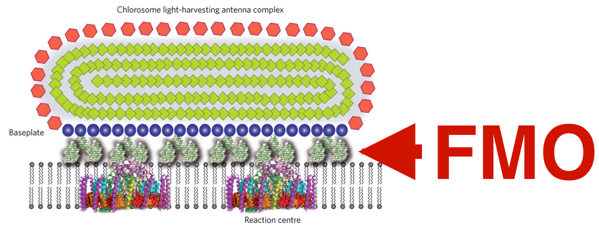
- Model dimers



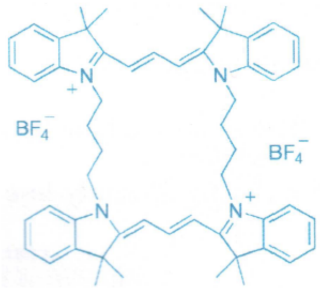
- Fenna-Mathews-Olson complex



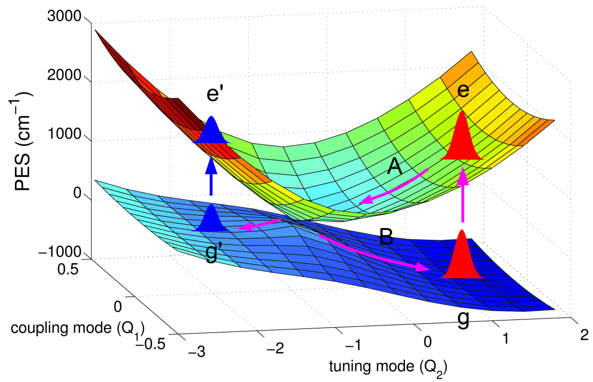
FMO complex



- Vibrational effects



- Conical intersections in wave packet propagation



Conclusions

- Open quantum systems: System-Bath Model
- Bath introduces dissipation & quantum decoherence / memory
- Numerically exact QUAsiadiabatic propagator Path Integral
- Path integral as a tensor network: TEMPO
- Applications:
  - Superconducting qubit coupled to readout device
  - sub-Ohmic heat bath
  - Quantum 1/f noise
  - Qubit coupled to non-commuting baths