The ACE project:

From numerically exact methods to modeling state-of-the-art experiments

technische universität dortmund

Ministerium für Kultur und Wissenschaft des Landes Nordrhein-Westfalen

Moritz Cygorek
Technische Universität Dortmund, Germany
Lisbon, 01. May 2026

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QOpen Many-body Open Quantum Systems

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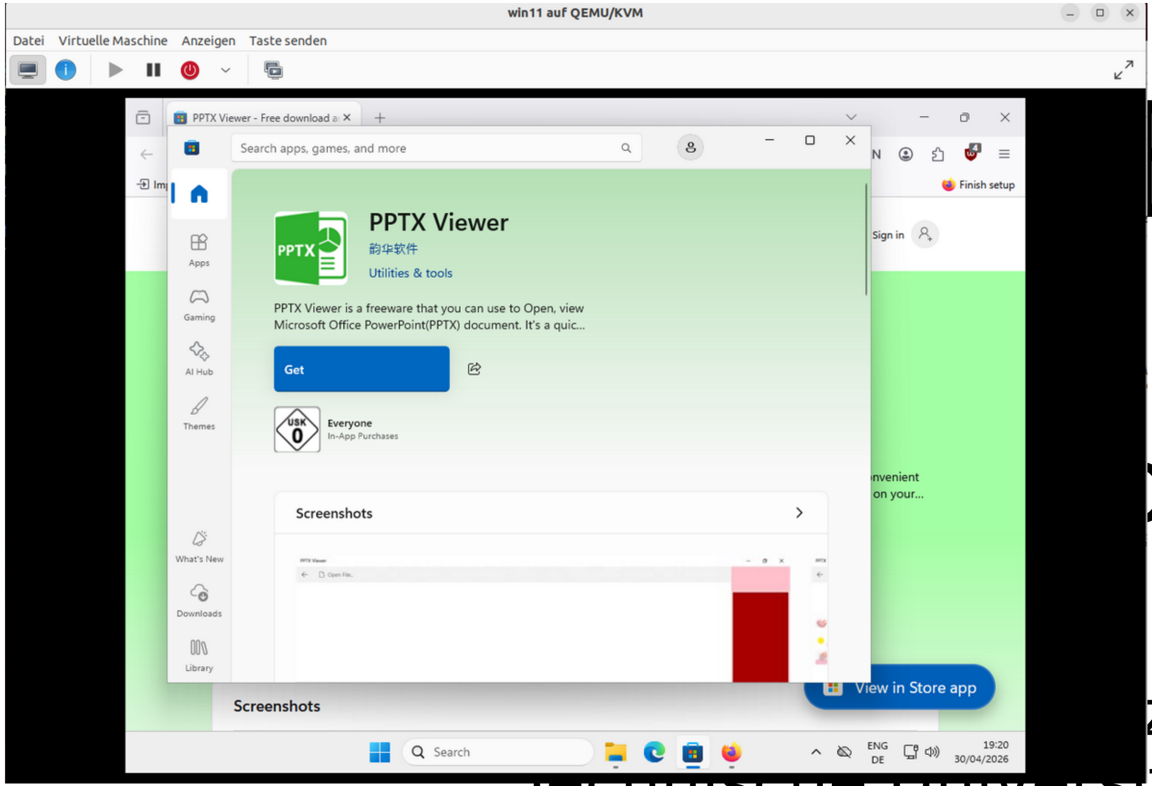

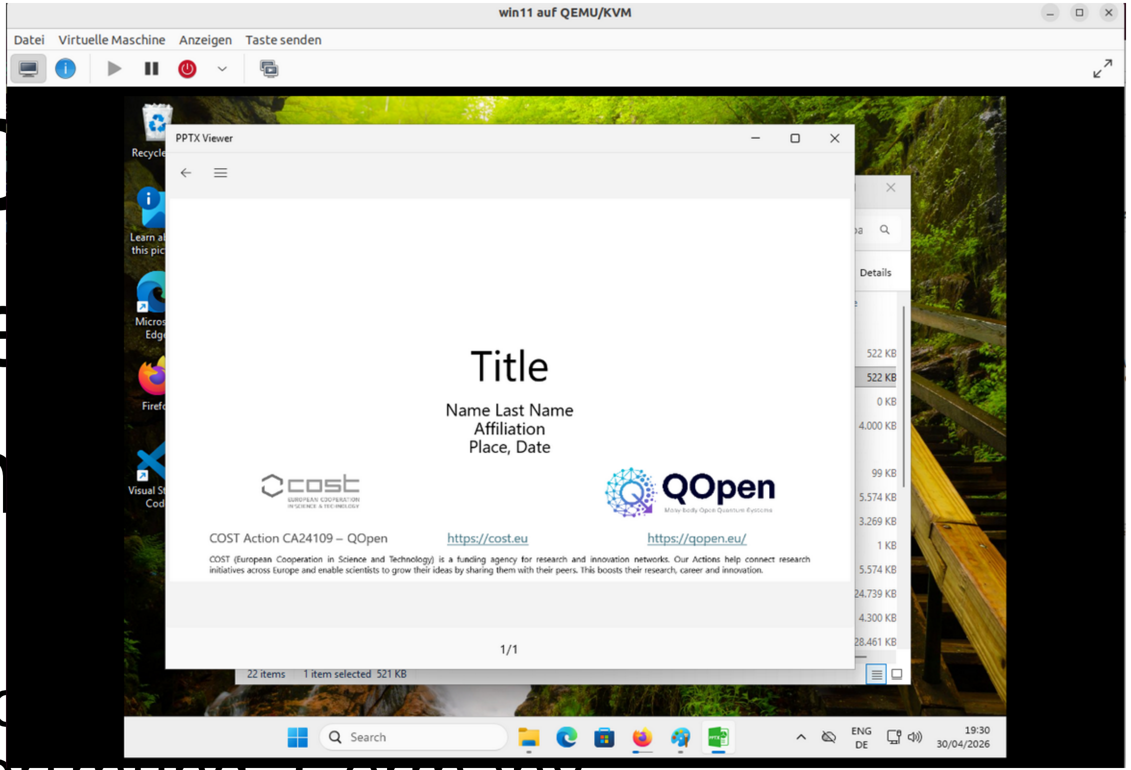

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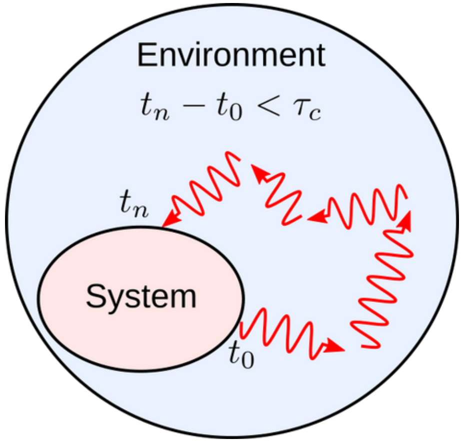
Open quantum systems



- Composite: System + Environment

$$H = H_S + H_E$$

- Formal solution:

$$\bar{\rho}(t) = \mathrm{Tr}_E\Big\{e^{-\frac{i}{\hbar}(H_S+H_E)t}\,\big(\bar{\rho}(0)\otimes\rho^E(0)\big)\,e^{\frac{i}{\hbar}(H_S+H_E)t}\Big\}$$

- Explicitly account for **environment degrees of freedom**

  ⇒ quantum many-body system

- Trace out environment

  ⇒ environment → **memory**

- Short memory (Markov)

  ⇒ Lindblad Master Equation

$$\dot{\rho} = -\frac{i}{\hbar}[H,\rho] + \sum_i \gamma_i \left(L_i\rho L_i^\dagger - \frac{1}{2}\left\{L_i^\dagger L_i, \rho\right\}\right)$$

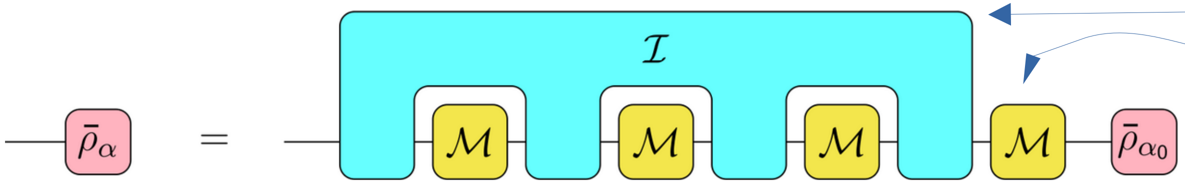
Process Tensors: Concept

$$\bar{\rho}(t) = \mathrm{Tr}_E\Big\{e^{-\frac{i}{\hbar}(H_S+H_E)t}\,\big(\bar{\rho}(0)\otimes\rho^E(0)\big)\,e^{\frac{i}{\hbar}(H_S+H_E)t}\Big\}$$

Time grid & Trotter decomposition

$$e^{-\frac{i}{\hbar}(H_S+H_E)t} = \prod_{l=1}^{n}\Big(e^{-\frac{i}{\hbar}(H_S+H_E)\Delta t}\Big) \qquad e^{-\frac{i}{\hbar}(H_S+H_E)\Delta t} = e^{-\frac{i}{\hbar}H_E\Delta t}e^{-\frac{i}{\hbar}H_S\Delta t} + \mathcal{O}(\Delta t^2)$$

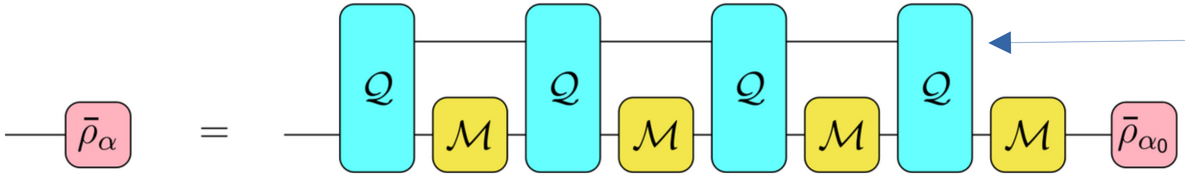
$$\bar{\rho}(t) \approx \mathrm{Tr}_E\Big\{e^{-\frac{i}{\hbar}H_E\Delta t}e^{-\frac{i}{\hbar}H_S\Delta t}e^{-\frac{i}{\hbar}H_E\Delta t}e^{-\frac{i}{\hbar}H_S\Delta t}\dots e^{-\frac{i}{\hbar}H_E\Delta t}e^{-\frac{i}{\hbar}H_S\Delta t}\big(\bar{\rho}(t_0)\otimes\rho^E(0)\big)\dots\Big\}$$



Influence functional

Free System Propagation

$\Downarrow$ Matrix Product Operator (MPO)



Process Tensor (PT-MPO)

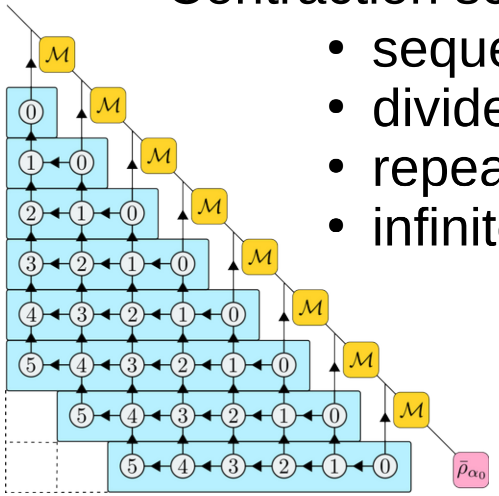
Process Tensors: Algorithms

(a) Gaussian

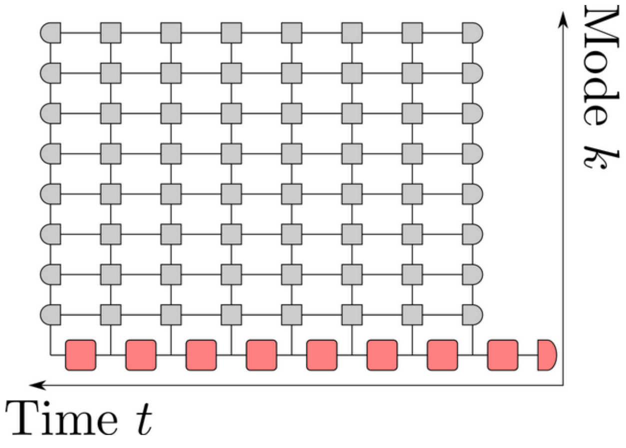
$$\mathcal{F}^{\alpha_n,\dots,\alpha_1} = \prod_{j=1}^{n}\prod_{l=0}^{n-j}[b_l]^{\alpha_{l+j},\alpha_j}$$

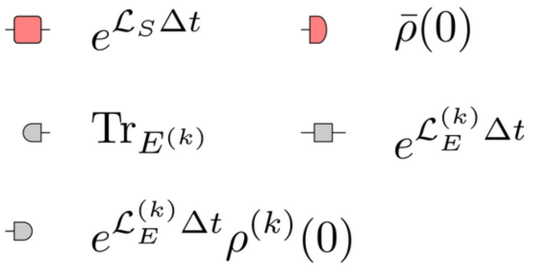
Contraction schemes:

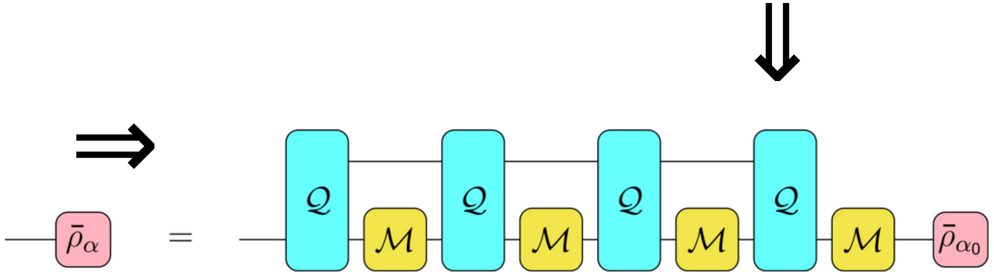
- sequential
- divide-and-conquer
- repeating blocks
- infinite MPOs



(b) independent modes







Automated **C**ompression of **E**nvironments

[Nature Physics 18, 662 (2022)]

ACE Code: Implemented methods

Path integrals (spin-boson):

(1963) Feynman & Vernon:
influence functional $O(N^{2n})$

(1991) Makri: QUAPI $O(N^{2m})$

(since 2011) Vagov & Axt: QUAPI for QDs

(2017) Cygorek, Barth, Axt:
Group decomposition $O(N N_g^{2m-2})$

MPO

Path integrals (spin-boson) + Tensor networks

(2018) Strathearn, Keeling & Lovett:
TEMPO: O(nm)

(2019) Jorgensen & Pollock: PT-MPO: O(nm)

(2024) Cygorek, Keeling, Lovett, Gauger:
divide-and-conquer: O(n log n)
periodic PT-MPOs: O(m log m)

ACE code

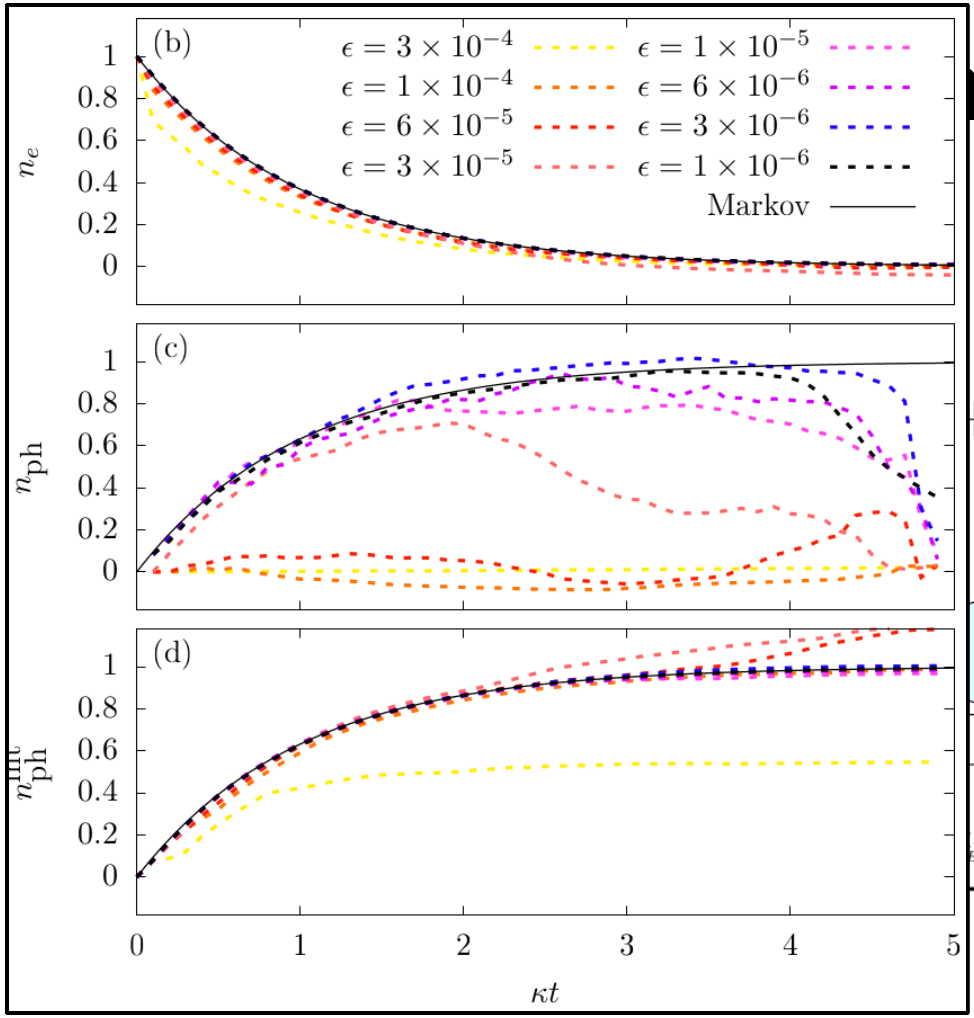
(2024) Link, Tu, Strunz: uniTEMPO: O(m)

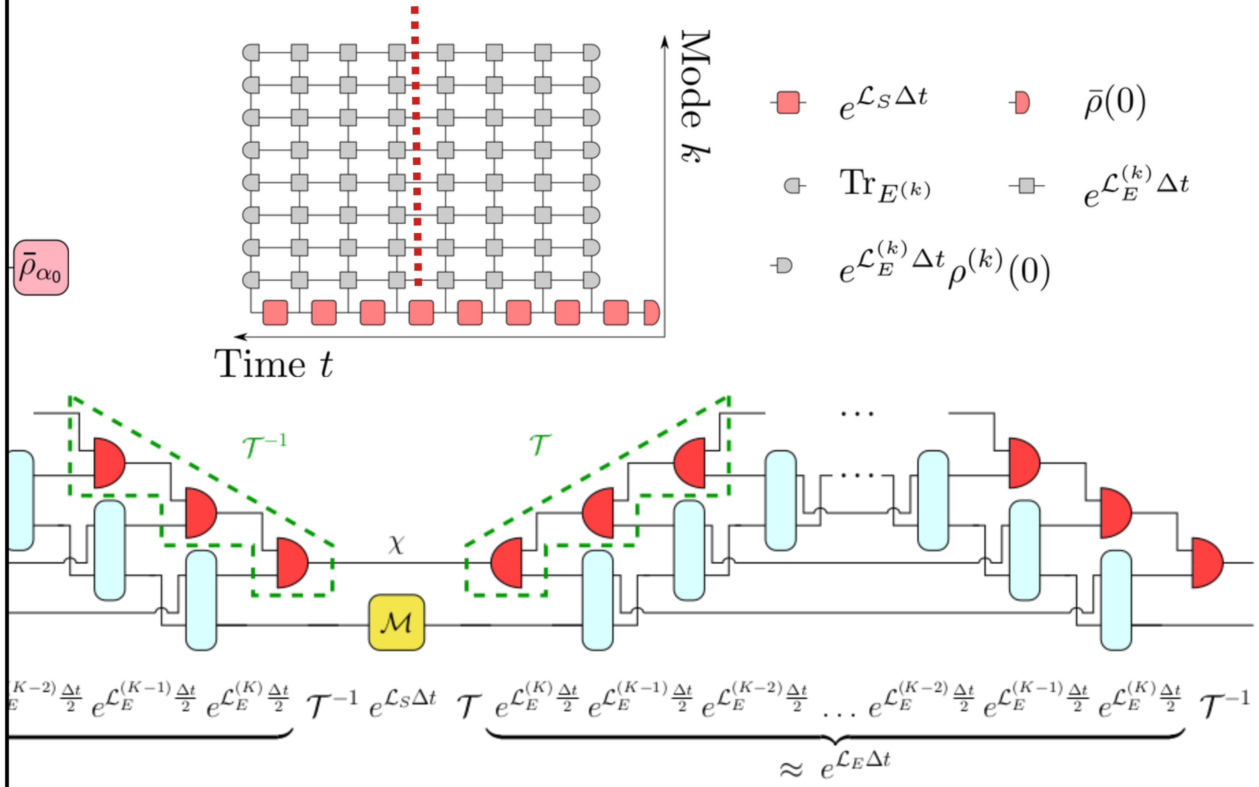
Independent modes:

(2022) Cygorek, Keeling, Lovett, Gauger: ACE

(2024) Cygorek, Keeling, Lovett, Gauger:
Tree-like ACE contraction

nterpretation of inner bonds





[Cygorek & Gauger, SciPost Phys. 18, 024 (2025)]

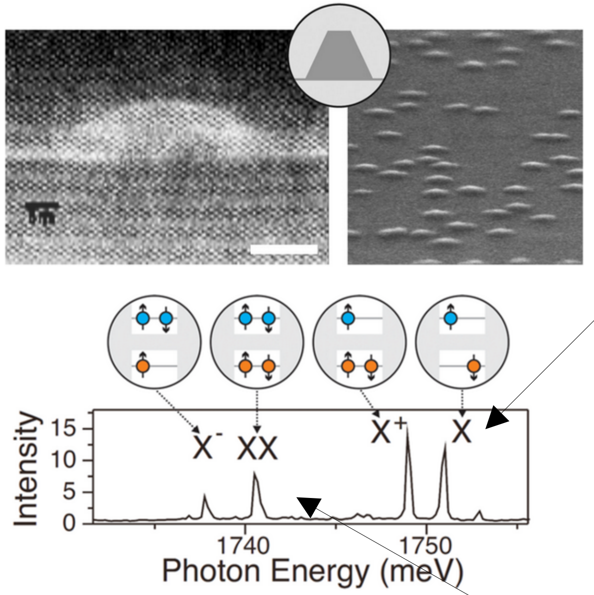
$\mathcal{Q} = \mathcal{T} e^{\mathcal{L}_E \Delta t} \mathcal{T}^{-1}$ = environment propagator compressed to the most relevant degrees of freedom

⇒ „Optimal Markovian embedding“

⇒ χ measures „non-Bornity“

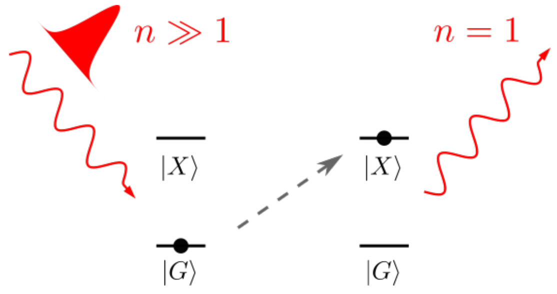
Applications: Semiconductor Quantum Dots

Epitaxial QDs

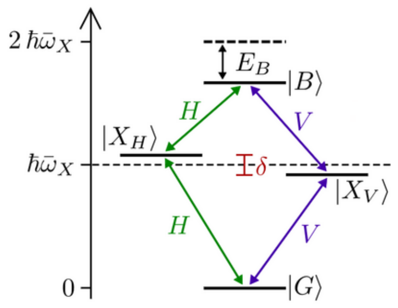


[Dietrich *et al.*,
Laser Photonics Rev. 10, 870 (2016)]

Single-photon source:

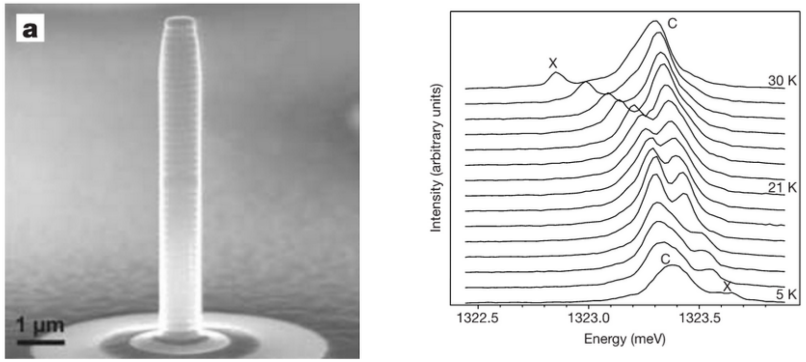


Entangled-photon source:



$$|\Psi\rangle = \frac{1}{\sqrt{2}}\big(|HH\rangle + |VV\rangle\big)$$

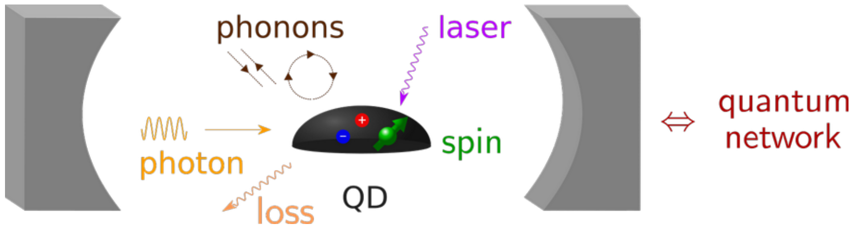
QDs in photonic structures



[Reithmaier *et al.*, Nature 432, 197 (2004)]

⇒ efficient light extraction (Purcell effect)

⇒ solid-state cavity-QED



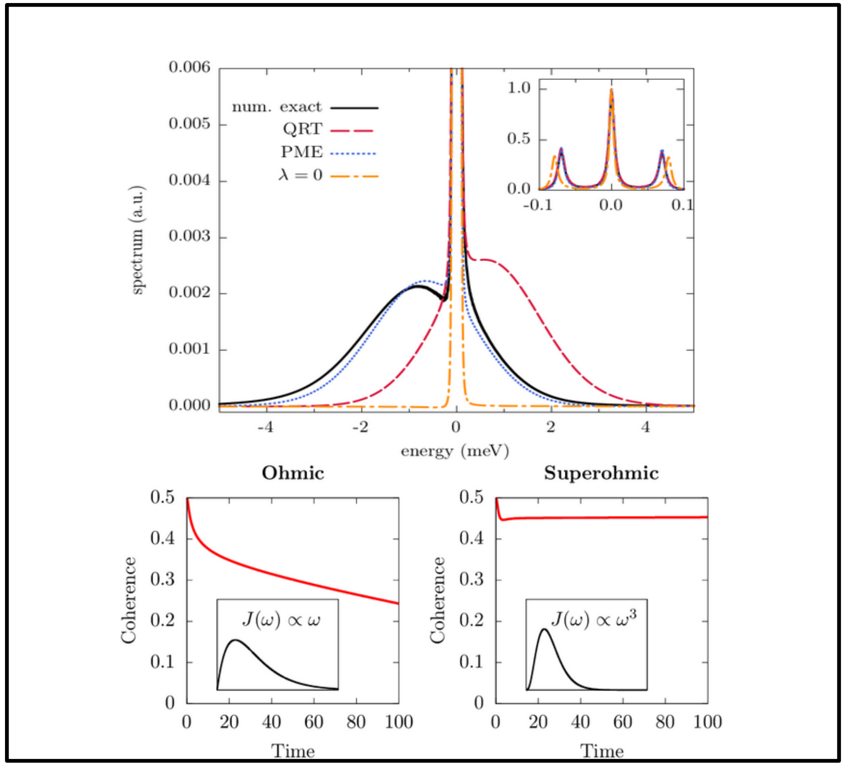
Quantum-Dot--Phonon Interaction

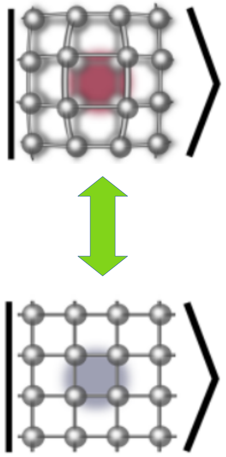
Electronic excitation in QD:

→ charge redistribution

→ reaction of crystal lattice

→ LA phonons





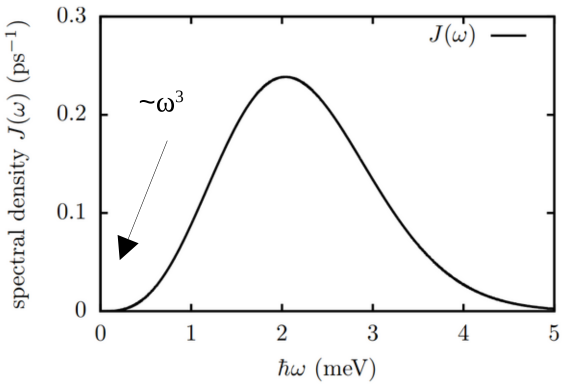
Spin-Boson interaction:

$$H_E = \sum_k \hbar\omega_k b_k^\dagger b_k + \sum_k \hbar g_k \left(b_k^\dagger + b_k\right)|X\rangle\langle X|$$

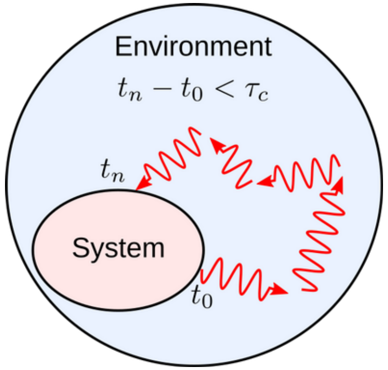
Spectral density: $J(\omega) = \sum_k |g_k|^2 \delta(\omega - \omega_k)$

For super-Ohmic QD-Phonon coupling:

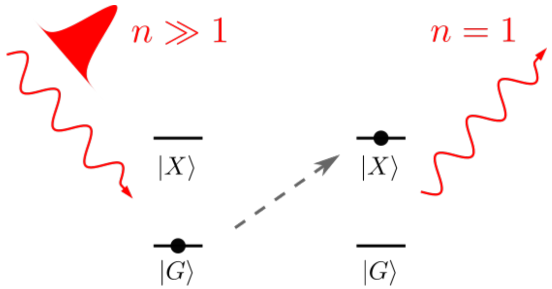
$$J^{\rm QD}(\omega) = \frac{\omega^3}{4\pi^2 \rho\hbar c_s^5}\left(D_c e^{-a_e^2\omega^2/(4c_s^2)} - D_h e^{-a_h^2\omega^2/(4c_s^2)}\right)^2$$

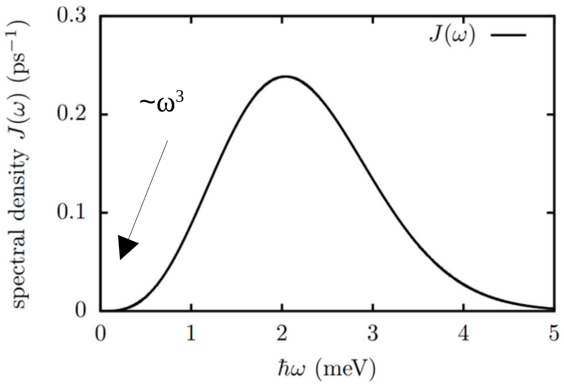


Memory: τ_c ~ 3-5 ps



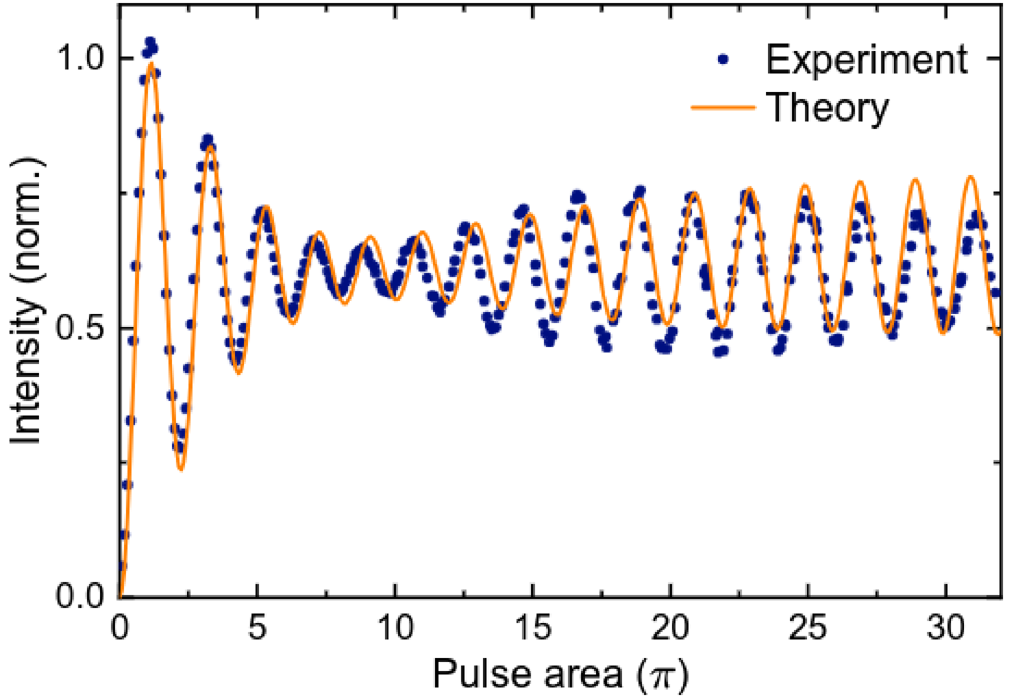
Applications: Single-photon sources





Reappearance of Rabi

[Hanschke *et al.*, Phys. Rev. Lett. 135, 263602 (2025)]

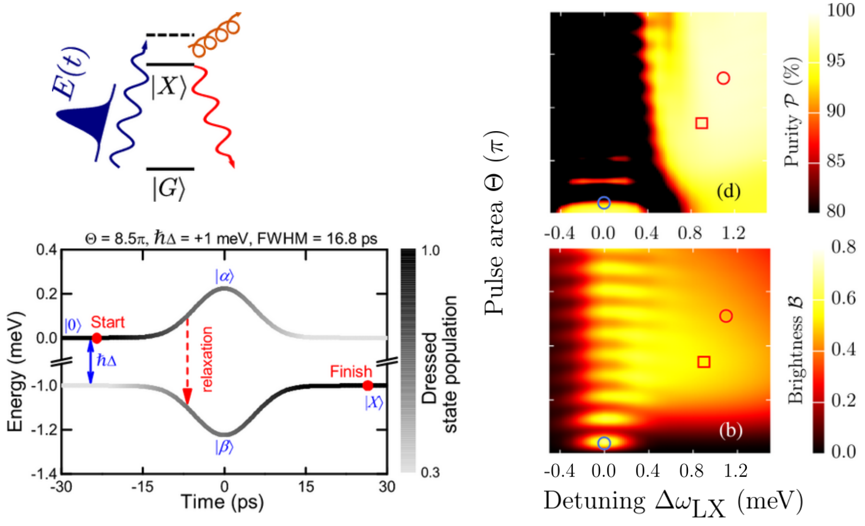


Applications: Single-photon sources

Issue: Resonant excitation scatters into output ⇒ Need efficient off-resonant excitation

Phonon-assisted excitation

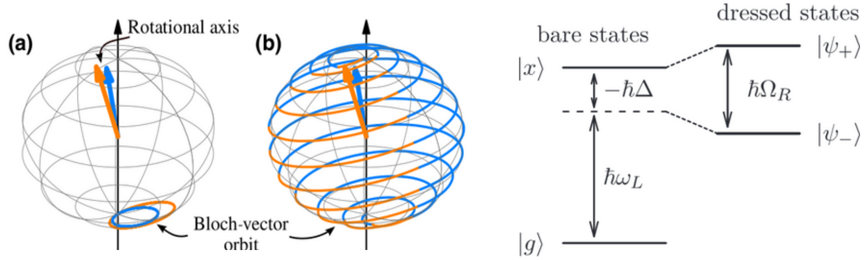
[Cosacchi et al., PRL 123, 017403 (2019)]



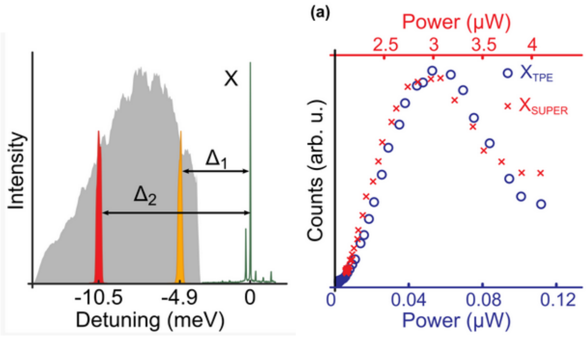
⇒ Phonons **help** achieve better/more robust state preparation

SUPER

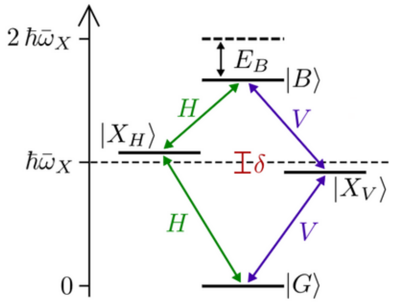
[Bracht *et al.*, PRX Quantum 2, 040354 (2021)]



[Karli *et al.*, Nano Letters 22, 6567 (2022)]

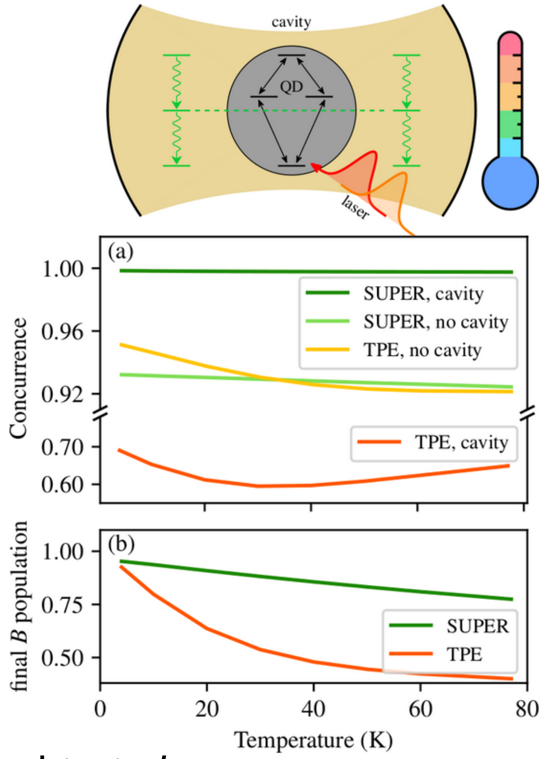


Applications: Multi-photon emission



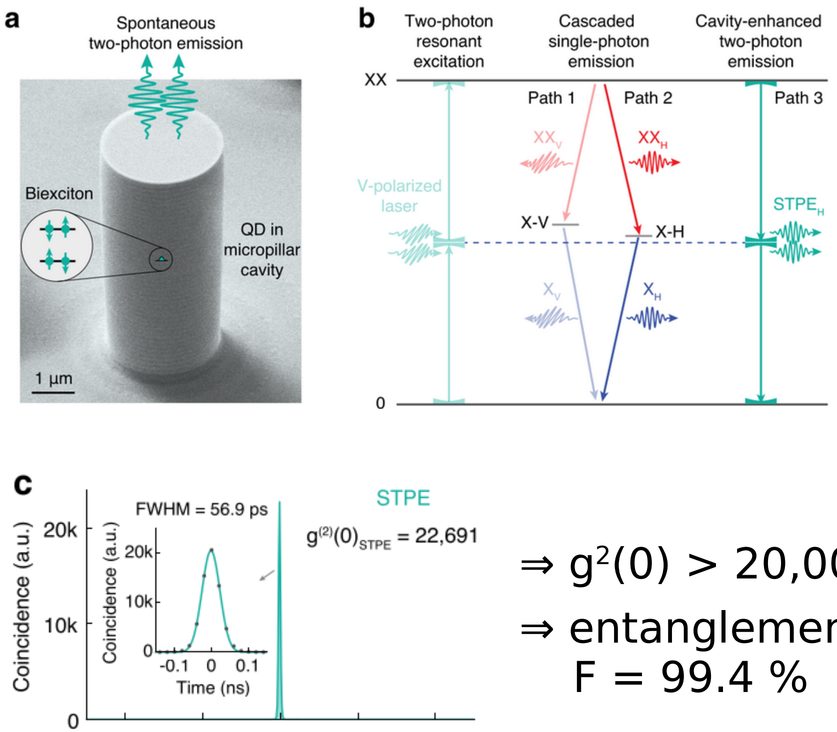
$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|HH\rangle + e^{i\delta t}|VV\rangle\right)$$

SUPER for BX in cavity



[Bracht *et al.*,
Optica Quantum 1, 103 (2023)]

Pure two-photon emission



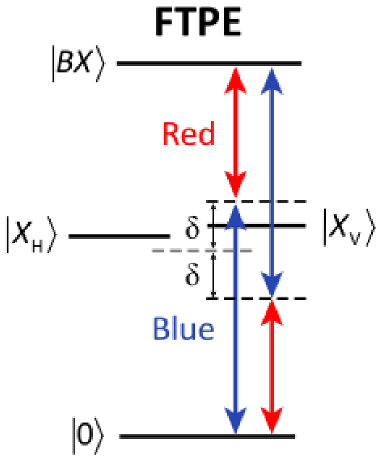
⇒ $g^2(0) > 20{,}000$

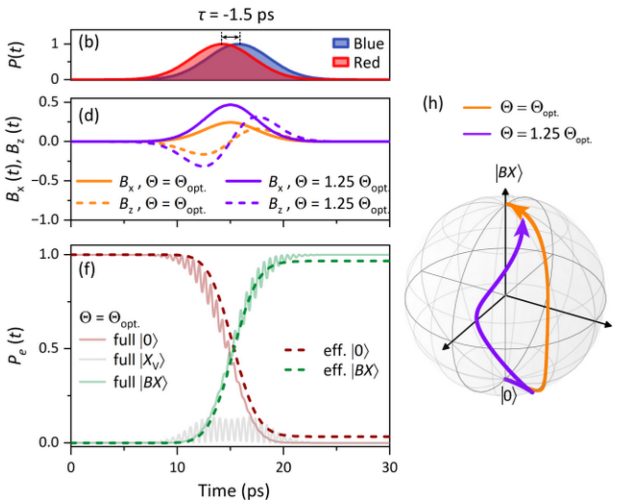
⇒ entanglement
F = 99.4 %

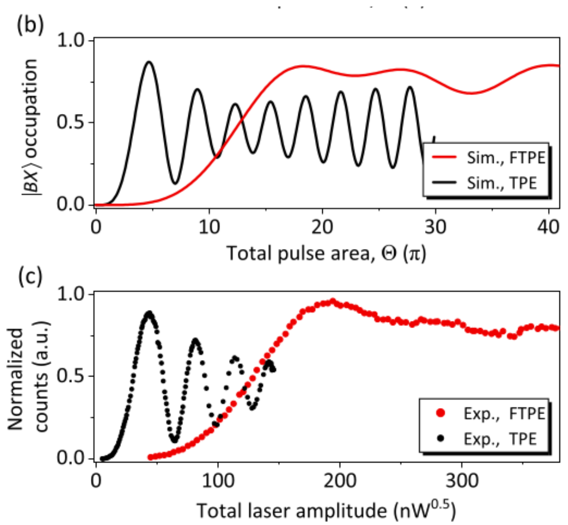
[with Jin Liu: Nature 643, 1234 (2025)]

Applications: Multi-photon emission

Single-shot Floquet driving







⇒ tunable stroboscopic Hamiltonian

⇒ robust biexciton preparation

[with Feng Liu: arxiv: 2504.02753v1]

$$\Omega(t) = f(t-\tfrac{\tau}{2})e^{-i\delta t} + f(t+\tfrac{\tau}{2})e^{i\delta t}$$

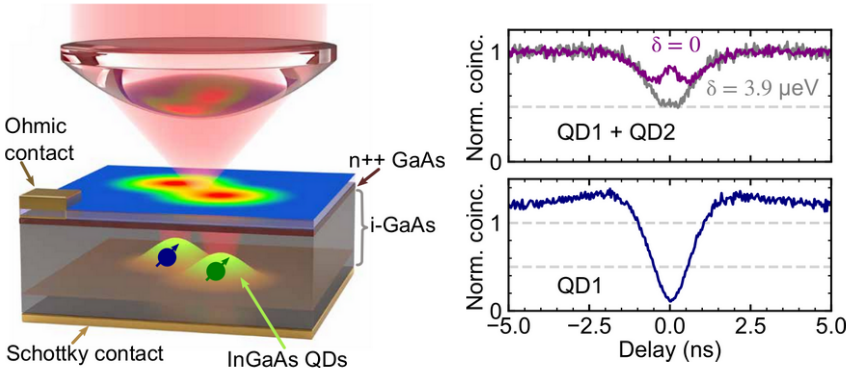
$$H/\hbar = \begin{pmatrix} 0 & \Omega^*(t)/2 & 0 \\ \Omega(t)/2 & E_b/(2\hbar) & \Omega^*(t)/2 \\ 0 & \Omega(t)/2 & 0 \end{pmatrix}$$

Floquet/Magnus →

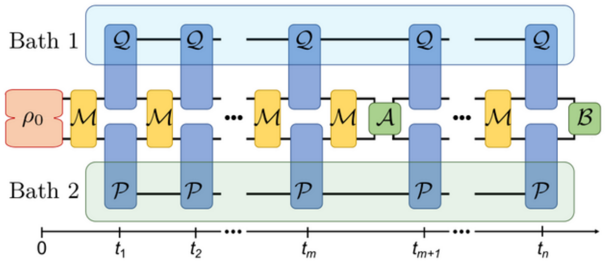
$$H^{\text{eff.}}(t) = \frac{\hbar}{2}\big(B_x(t)\sigma_x + B_z(t)\sigma_z\big)$$

Applications: Cooperative emission

Measurement-induced collective emission

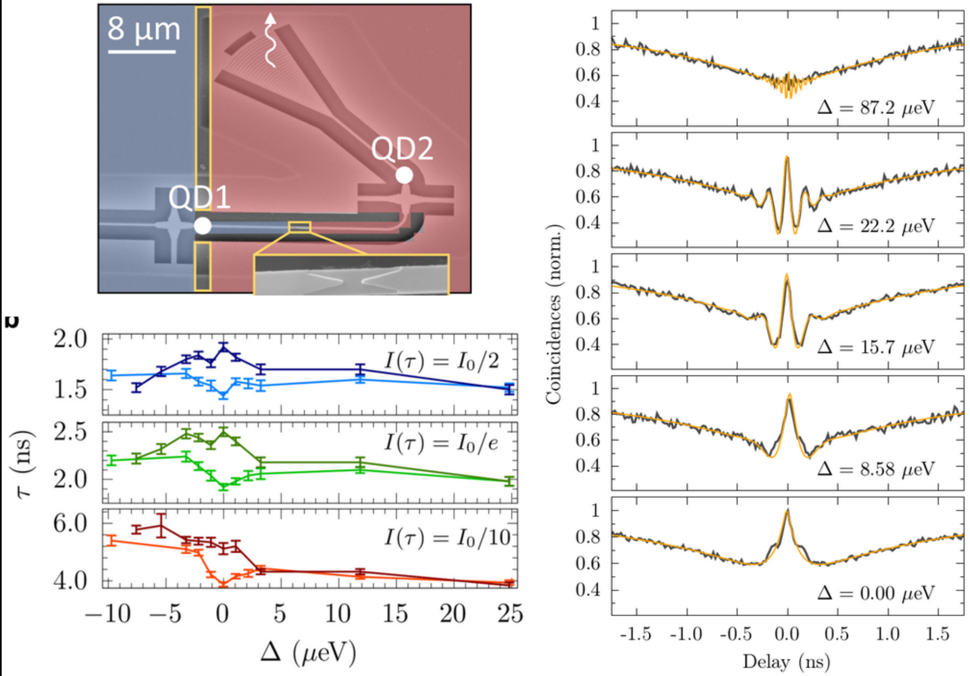


[Koong *et al.*, Sci. Adv. 8, eabm8171 (2022)]



[Wiercinski *et al.*, Phys. Rev. Research 5, 013176 (2023)]

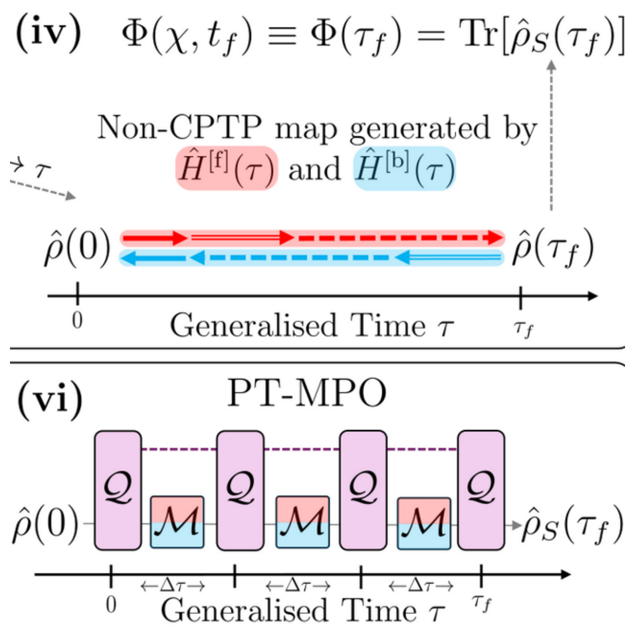
Superradiance



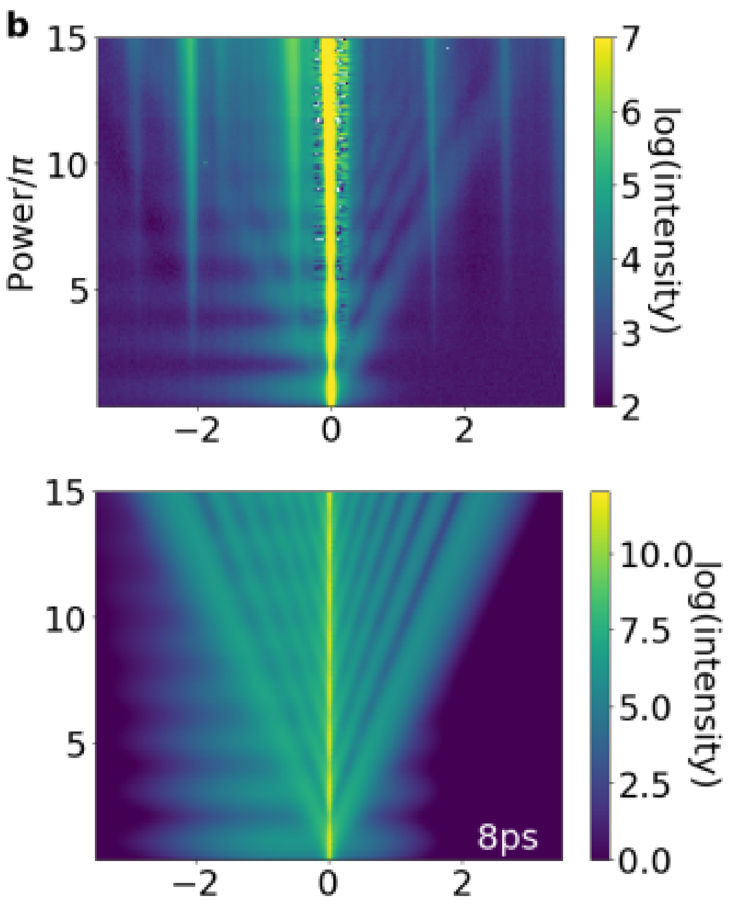
[Hallett *et al.*, Phys. Rev. Applied 25, L021003 (2026)]

Other Applications

- Dynamical dressing / pulsed Mollow spectra
- Quantum Thermodynamics
- Transport
- ...

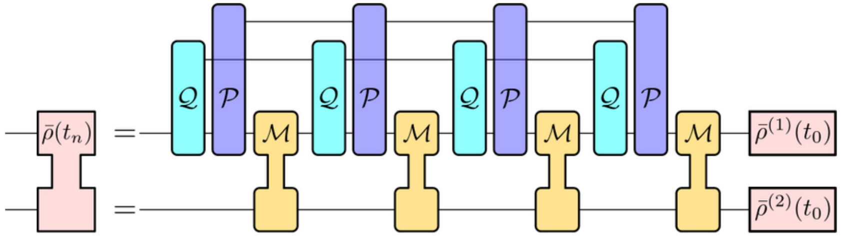


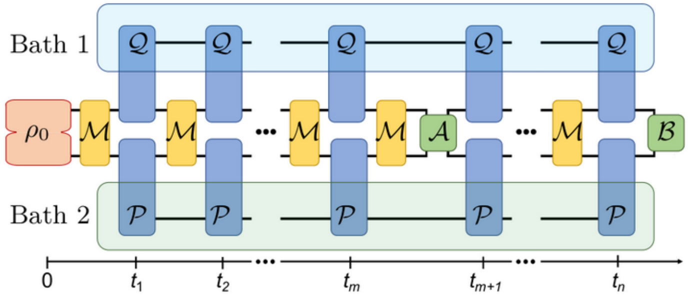
[Shubrook *et al.*, arXiv:2512.16823v1 (2025)]



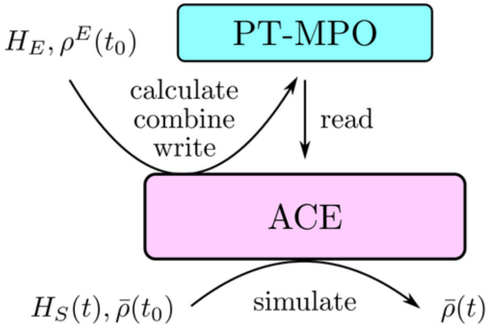
[Boos *et al.*, PRL 132, 053602 (2024)]

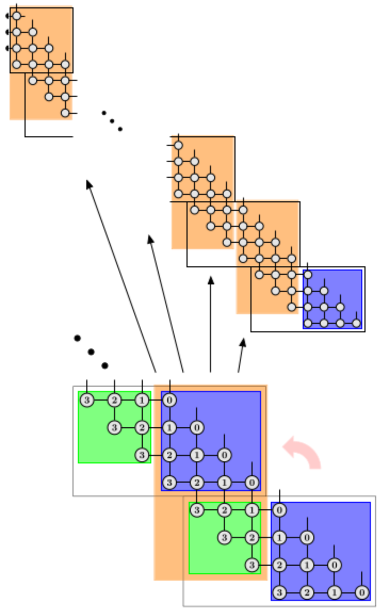
Recent advances





- **Multiple levels & Composite systems**
  [QD in cavity $(4\text{x}3\text{x}3)^2 = 1296$]
- **Multiple environments**
  [products of inner bonds ⇒ exponential scaling]
- Ultrafast driving <100 fs
  but overall dynamics > 1ns
  ⇒ **10^4 … 10^6 time steps**
- Very general scope ⇒ code has to be **versatile**
- …





The ACE Code: C/C++ Codebase

- High numerical demands:

  ⇒ explicit resource handling

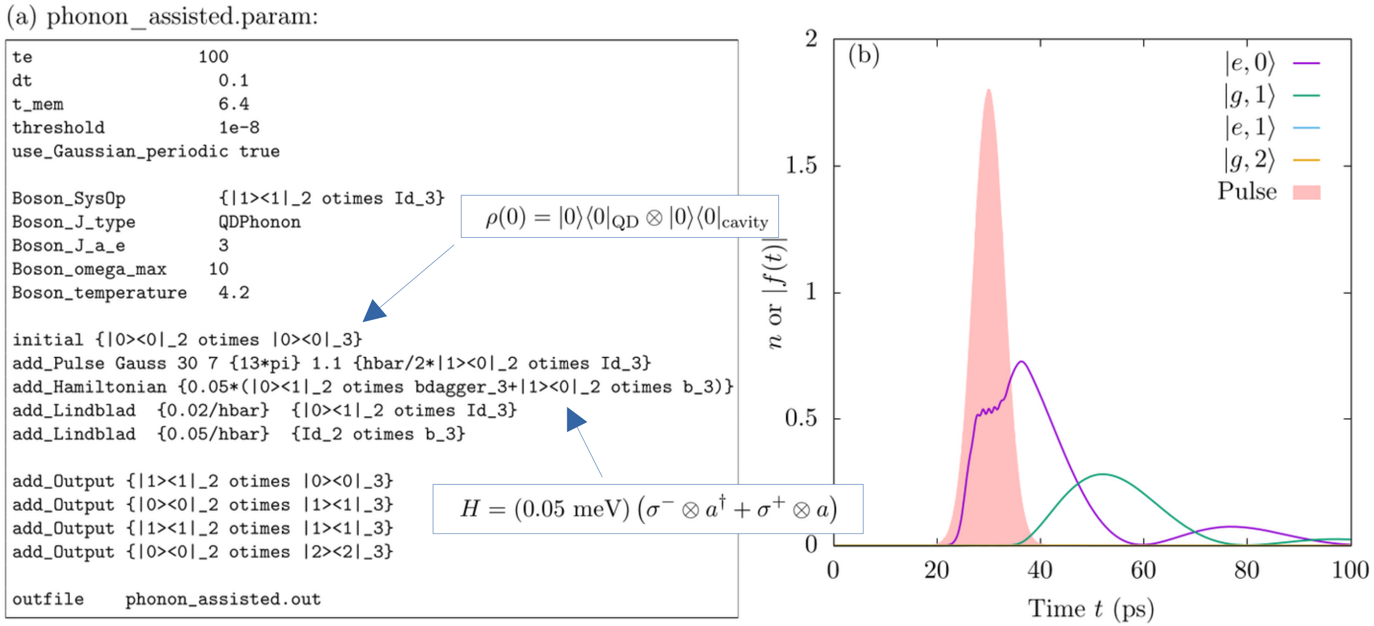
  ⇒ high-performance computing

  ⇒ BLAS/LAPACK/MKL

- Parameter files:

  ⇒ Concise language for defining quantum systems & interactions

  ⇒ no programming required



The ACE Code: Python

- Python is common and easy to learn
- Python bindings access C/C++ library

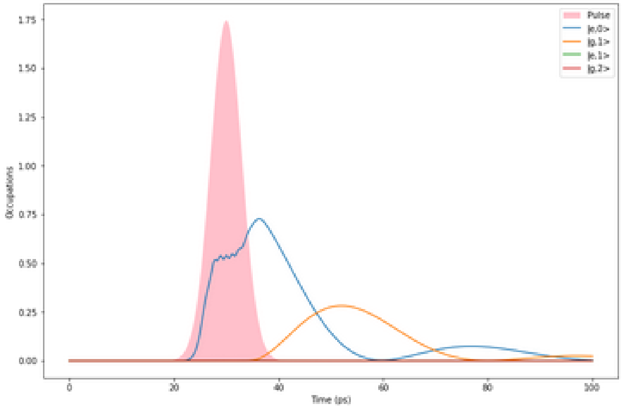
⇒ Combine userfriendliness
with speed and HPC!

Since last week: **CICD**
(Continuous integration, continuous delivery)

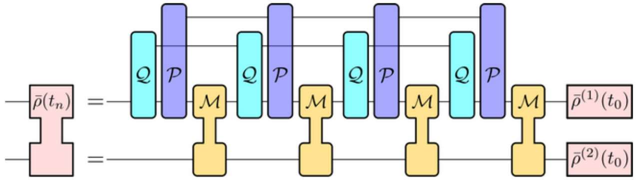
github → releases → Python wheels

> > pip install ACE-OQS

```python
from ACE import *
import numpy as np

# Parameters
te = 100   # end time
dt = 0.1   # time step
bdim = 3   # truncated dimension of cavity mode
T = 4.2    # temperature
g     = 0.05/hbar  # QD-cavity coupling (meV -> ps^-1)
gamma = 0.02/hbar  # radiative decay
kappa = 0.05/hbar  # cavity loss

# Gaussian pulse
def myPulse(t) -> complex:
    A     = 13        # pulse area (pi)
    tc    = 30        # pulse center (ps)
    FWHM  = 7         # pulse duration (ps)
    delta = 1.1/hbar # Detuning (meV -> ps^-1)
    sigma = FWHM/(2*np.sqrt(2*np.log(2)))
    return (A*np.pi)/(np.sqrt(2.*np.pi)*sigma)*np.exp(-0.5*((t-tc)/sigma)**2) * np.exp(-1j*delta*(t-tc))

# Define driving Hamiltonian:
pulseTimes = np.arange(0, te, dt/2, dtype=float)
pulseShape = ( pulseTimes, myPulse(pulseTimes) )
dipole = hbar/2*np.kron( KetBra(1,0,2), np.eye(bdim) )   # <- Kronecker product with identity matrix

H_JC = hbar*g*(np.kron(KetBra(0,1,2), Boson_create(bdim)) +   # <- Jaynes-Cummings coupling
               np.kron(KetBra(1,0,2), Boson_destroy(bdim)) )

# Define free system propagator and OutputPrinter
fprop    = FreePropagator()
fprop.add_Pulse( pulseShape, dipole )
fprop.add_Hamiltonian( H_JC )
fprop.add_Lindblad( gamma, np.kron(KetBra(0,1,2), np.eye(bdim)) )
fprop.add_Lindblad( kappa, np.kron(np.eye(2), Boson_destroy(bdim)) )

PT = ProcessTensors()
PT.add_PT(f'QDPhonon_T{T}_dt{dt}.pt', 0, bdim)

outp  = OutputPrinter( [np.kron( KetBra(1,1,2), KetBra(0,0,bdim) ),    # Observables: |e,0> occupations
                        np.kron( KetBra(0,0,2), KetBra(1,1,bdim) ),    # |g,1> occupations
                        np.kron( KetBra(1,1,2), KetBra(1,1,bdim) ),    # |e,1> occupations
                        np.kron( KetBra(0,0,2), KetBra(2,2,bdim) )])   # |g,2> occupations

Simulation(fprop, PT, np.kron( KetBra(0,0,2), KetBra(0,0,bdim) ), TimeGrid(0, te, dt), outp)
(times, data) = outp.extract()

# Now, plot the results:
import matplotlib.pyplot as plt
fig, ax = plt.subplots(1,1,figsize=(12,8))
ax.set(xlabel="Time (ps)")
ax.set(ylabel="Occupations")
ax.fill(pulseShape[0], np.abs(pulseShape[1])/(np.pi), 'pink', label='Pulse')
ax.plot(times, data[:,0].real, label='|e,0>')
ax.plot(times, data[:,1].real, label='|g,1>')
ax.plot(times, data[:,2].real, label='|e,1>')
ax.plot(times, data[:,3].real, label='|g,2>')
ax.legend(loc="upper right")
plt.show()
```



Current challenges



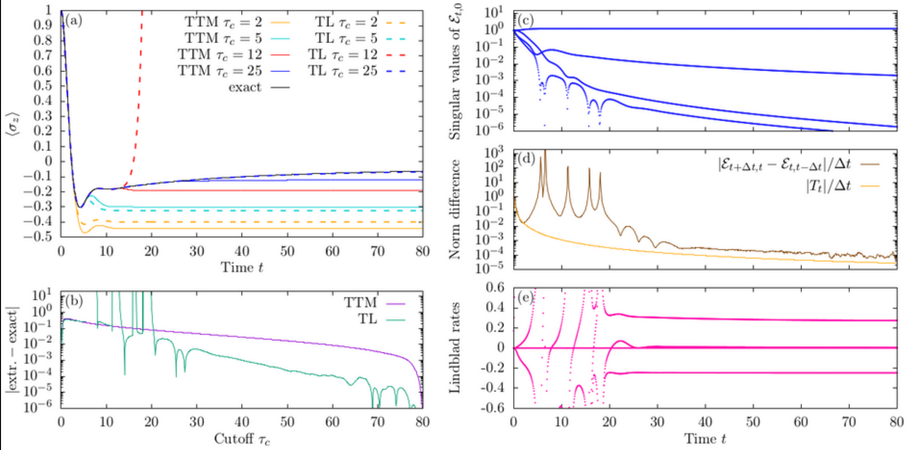
- Large systems
- “Incompressible” environments
- Interacting environment modes
- …

$$e^{-\frac{i}{\hbar}H_S\Delta t}$$

$$\mathcal{Q} = \mathcal{T} e^{\mathcal{L}_E \Delta t}\mathcal{T}^{-1}$$

Time-local dynamical maps

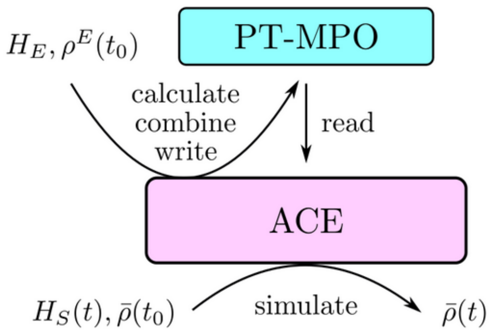
$$\rho_{t_n} = \mathcal{E}_{t_n,t_0}\rho_{t_0} \quad \Rightarrow \quad \mathcal{E}_{t_n+\Delta t,t_n} = \mathcal{E}_{t_{n+1},t_0}\mathcal{E}^{-1}_{t_n,t_0}$$

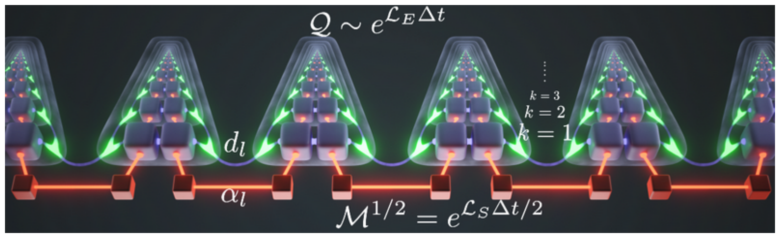


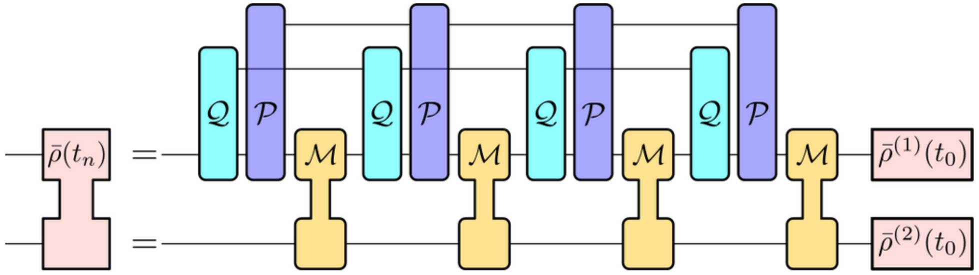
[arXiv:2505.21017]

Summary:

- ACE = fast, versatile, and userfriedly simulator for (non-Markovian) open quantum system
- Proven success in modeling state-of-the-art experiments
- Main challenges identified; some addressed, some under investigation







https://github.com/mcygorek/ACE →