

Reaction Coordinate Master Equation for Transport Problems Beyond Born-Markov

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Outline

1 Primer on Open Quantum System

2 Master Equations

- Lindblad Equation
- Bloch-Redfield Equation
 - Aside: secular approximation

3 Reaction Coordinate Master Equation

- Non-equilibrium spin-boson
- Quantum Absorption Refrigerator
- Quantum transport beyond second order
- Effective Hamiltonian Theory at strong coupling
- Markovian dynamics

4 Outlook

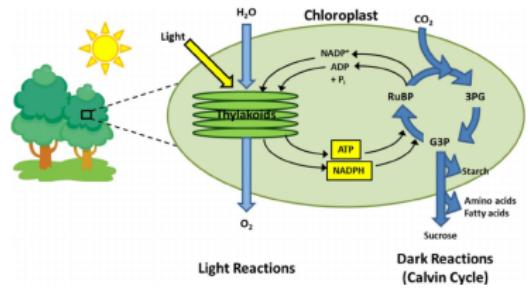
Question 1

How would a **quantum** system evolve in contact with a thermal environment?

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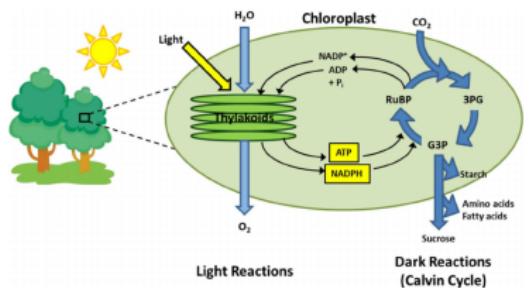
How would a **quantum** system evolve in contact with a thermal environment? ← Why is this interesting?

Quantum systems in contact with a thermal bath (in nature)



- Photosynthesis is at room temperature

Quantum systems in contact with a thermal bath (in nature)



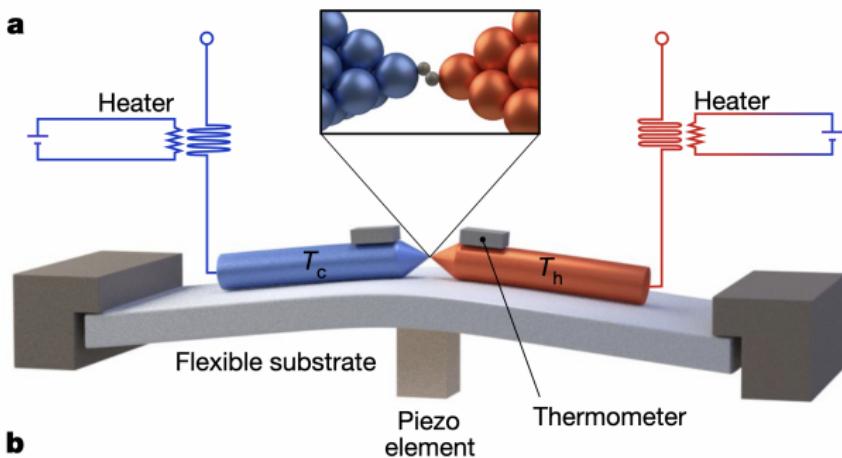
- Photosynthesis is at room temperature
- Quantum effects in photosynthesis

Quantum biology...

The image displays a collage of scientific publications from 2010 and 2011, illustrating the field of quantum biology:

- PNAS (top left):** An article titled "Quantum entanglement in photosynthetic light-harvesting complexes" by Mohan Sarovar, Akihito Ishizuka, and K. Birgitta Whaley, published online on April 25, 2010. DOI: 10.1073/pnas.100503.
- Physical Review Letters (center left):** An article titled "Sustained Quantum Coherence and Entanglement in the Avian Compass" by Erik M. Gauger, Elisabeth Rieper, John I. L. Morton, Simon C. Benjamin, and Vladko Vedral, published online on April 25, 2010. DOI: 10.1103/PhysRevLett.106.040503.
- Nature Physics (center top):** An article titled "Evidence for wavelike energy transfer through quantum coherence in photosynthetic systems" by Gregory S. Engel, Tessa R. Calhoun, Yuan-Chung Cheng, Robert E. Blankenship, and Stuart M. Olson, published online on April 25, 2010. DOI: 10.1038/nphys1652.
- Science (bottom right):** An article titled "Coherent Control of Retinal Isomerization in Bacteriorhodopsin" by Heth L. Read, Tae-Kyu Ahn, Tomoaki Saito, Graham R. Fleming, and David J. Deamer, published online on April 24, 2010. DOI: 10.1126/science.1190578.

Quantum systems in contact with a thermal bath (...in the lab)



- Atomic junction experiments¹
- Quantum system as a conductor

¹Ofir Shein Lumbroso, Lena Simine, Abraham Nitzan, Dvira Segal, and Oren Tal,
Nature 2018

How would a **quantum** system evolve in contact with a thermal environment?

- **Quantization?** Feynman: thermal environment → infinitely many harmonic oscillators.

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But...

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But... Dirac:

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But... Dirac:

- ...laws necessary for the ...large part of physics and the whole of chemistry are thus completely known,
- ... the difficulty is only that the **exact** application of these laws leads to equations much too complicated to be soluble...

i.e., $|\psi_{S+E}(t)\rangle$ is huge **but** we do not care about the environment part.
One solution is to use a dissipative master equation.

Lindblad equation: Top-Down (short time expansion of the Kraus operator)

The reduced system density matrix satisfies

$$\langle i | \rho | i \rangle \geq 0 \quad (1)$$

$$\text{Tr}\{\rho\} = 1 \quad (2)$$

Therefore, we'd like to find a quantum map that preserves these properties,

$$\rho \rightarrow \rho', \text{ via } \dot{\rho} = \mathcal{L}\rho \quad (3)$$

²Breuer and Petruccione or Lidar are good references

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which Lindblad proved to take the general GKLS form²

$$\dot{\rho} = \underbrace{-i[\hat{H}, \rho]}_{\text{unitary}} + \underbrace{\sum_k \Gamma_k \left(L_k \rho L_k^\dagger - \frac{1}{2} \{ L_k^\dagger L_k, \rho \} \right)}_{\text{dissipator}} \equiv \mathcal{L}\rho. \quad (4)$$

²Breuer and Petruccione or Lidar are good references

Master Equations: Bottom-up (perturbative)

Schrodinger's Equation



Von Neumann



Born-Markov, Tr_B

Redfield QME



Secular

Lindblad QME

Lindblad is Secular Redfield

The bottom up derivation of Lindblad equation is Redfield (Born-Markov) + Rotating Wave (Secular) Approximation.

We will stop at Redfield to go beyond secular, but note that Redfield is notoriously non-CPTP.

Born-Markov Redfield: Primer

The full Hamiltonian takes the form

$$\hat{H} = \underbrace{\hat{H}_S + \hat{H}_B}_{\hat{H}_0} + \hat{V}, \quad (5)$$

with

$$\hat{H}_B = \sum_j \omega_j \hat{b}_j^\dagger \hat{b}_j. \quad (6)$$

The system-bath interaction Hamiltonian is bilinear

$$\hat{V} = \hat{S} \otimes \hat{B}; \quad \hat{B} = \sum_j g_j (\hat{b}_j^\dagger + \hat{b}_j). \quad (7)$$

g_j describes the system-bath coupling energy between mode j in the bath and the system.

Born-Markov Redfield: Derivation Sketch

- Starting from von Neumann equation in the interaction picture,

$$\dot{\rho}_I(t) = -i[\hat{V}_I, \rho_I(t)] \quad (8)$$

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$$\dot{\rho}_I(t) = -i[\hat{V}_I, \rho_I(t)] \quad (8)$$

- Make the **Born** approximation, i.e., $\rho \approx \rho_S \otimes \rho_B$ and " $\hat{V} \ll \hat{H}_0$ "

$$\underbrace{\frac{\partial \rho_I}{\partial t}(t) = -i[\hat{V}_I(t), \rho_I(t_0)] - \int_{t_0}^t d\tau [\hat{V}_I(t), [\hat{V}_I(\tau), \rho_I(\tau)]]}_{\text{Partial trace } \Rightarrow \frac{\partial \rho_{S,I}}{\partial t}(t) = \underbrace{-i \text{Tr}_B \{ [\hat{V}_I(t), \rho_I(t_0)] \}}_{0 \text{ for a harmonic bath}} - \text{Tr}_B \{ \int_{t_0}^t d\tau [\hat{V}_I(t), [\hat{V}_I(\tau), \rho_I(\tau)]] \}}$$

Born-Markov Redfield: Derivation Sketch

- **Markov I** (also stationary bath)

$$\frac{\partial \rho_{S,I}(t)}{\partial t} = -\text{Tr}_B \left\{ \int_{t_0}^t d\tau [\hat{V}_I(t), [\hat{V}_I(\tau), \rho_{S,I}(\textcolor{red}{t}) \otimes \rho_B]] \right\}, \quad (10)$$

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- **Markov II:**

$$\frac{\partial \rho_{S,I}(t)}{\partial t} = -\text{Tr}_B \left\{ \int_0^\infty d\tau [\hat{V}_I(t), [\hat{V}_I(t-\tau), \rho_{S,I}(t) \otimes \rho_B]] \right\}. \quad (11)$$

Markov: memoryless, "What happens next depends only on the state of affairs now.". For example, drunkard's walk **is** Markov but Bus waiting is **not** Markov.

Born-Markov Redfield: Derivation Sketch

Rotate back to the Schrödinger picture and do algebra.

$$\frac{\partial \rho_s}{\partial t} = -\frac{i}{\hbar} [\hat{H}_s, \rho_s] - \int_0^\infty \left\{ [\hat{S}, e^{-i\hat{H}_s\tau} \hat{S} e^{i\hat{H}_s\tau} \rho_s(t)] \langle \hat{B}_I(t-\tau) \hat{B}_I(t) \rangle \right. \\ \left. - [\hat{S}, \rho_s(t) e^{-i\hat{H}_s\tau} \hat{S} e^{i\hat{H}_s\tau}] \langle \hat{B}_I(t) \hat{B}_I(t-\tau) \rangle \right\} d\tau \quad (12)$$

we'll eventually need to Laplace transform the bath correlation function

$$\underbrace{R_{ij,kl}(\omega)}_{\text{for Redfield Liouvillian}} = S_{ij} S_{kl} \int_0^\infty d\tau e^{i\omega\tau} \underbrace{\langle \hat{B}_I(\tau) \hat{B}_I(0) \rangle}_{\sum_j \lambda_j^2 [e^{i\omega_j t} \langle \hat{n}(\omega_j) \rangle + e^{-i\omega_j t} \langle \hat{n}(\omega_j) + 1 \rangle]} \quad (13)$$

The Sokhotski–Plemelj theorem says

$$\lim_{\epsilon \rightarrow 0^+} \frac{1}{x \pm i\epsilon} = \mp i\pi \delta(x) + \mathcal{P}\left(\frac{1}{x}\right), \quad (14)$$

Spectral Density

The real part of the Laplace transform $\Gamma(\omega)$ matters. (the imaginary part is a negligible Lamb shift). Notice that we'll find a delta term

$$\Gamma_\alpha(\omega) = \begin{cases} \pi J_\alpha(\omega) n_\alpha(|\omega|) & \omega < 0, \\ \pi J_\alpha(\omega)[(n_\alpha(\omega) + 1] & \omega > 0, \\ \pi C_\alpha & \omega = 0, \end{cases} \quad (15)$$

$$J(\omega) = \sum_k \lambda_k^2 \delta(\omega - \omega_k), \quad (16)$$

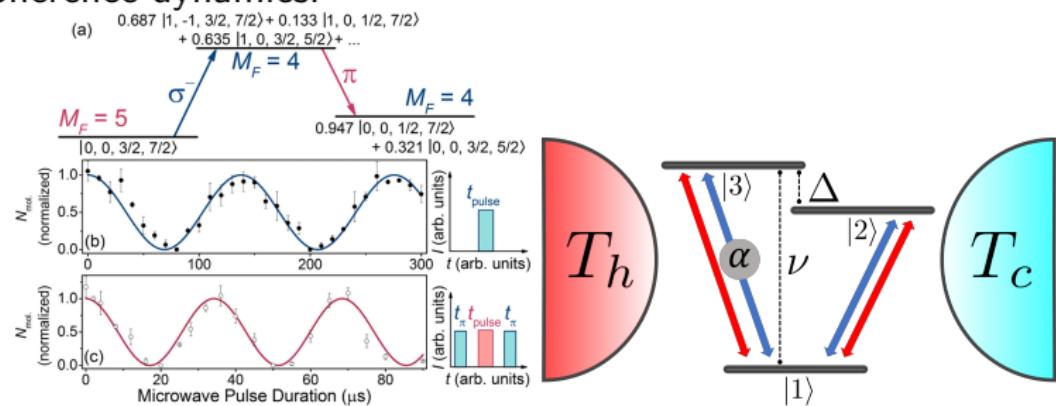
all we need to know about the environment is encoded in the spectral density $J(\omega)$.

Some remarks on Born-Markov Redfield QME

- Redfield QME is used all the time, especially for complex problems where microscopic details are important, e.g., in quantum thermodynamics, quantum biology, etc.
- Assumptions:
 - Born (Weak coupling) → second order in the system bath coupling parameter
 - Markov (Memoryless)
- But, unlike Lindblad, there is no secular approximation

Secular approximation

Fails for systems with near-degenerate levels, such as those used for (1) adiabatic quantum computing, (2) coherent population trapping and electromagnetically induced transparency, where coherences are prominent^{3,4}. This is because secular approximation decouples population and coherence dynamics.



³Fl, Nicholas Anto-Sztrikacs, and Dvira Segal, NJP 2022

⁴Fl, Nicholas Anto-Sztrikacs, and Dvira Segal, arxiv:2301.06135, 2023

Question 2:

How to go beyond Born-Markov?

- Fully Numerical:
 - Multiconfiguration time-dependent Hartree (MCTDH)
 - Hierarchical equations of motion (HEOM) (Tanimura)
 - Density matrix renormalization group (DMRG)
 - Numerical path integral (Segal, Millis, and Reichman, 2010 PRB) ← in the journal club suggestion list
 - **Chain-mapping methods**, particularly TEDOPA (Chin and Plenio)
 - Tensor network methods (Cao, Huelga, Plenio)
 - Quantum monte-carlo

i.e., solve cleverly the $S + B$ full dynamics.

Question 2:

- Inexact analytical:

- Non-interacting blip approximation (NIBA) (Segal)
- Polaron-transformation (Cao, Segal, Silbey, Cheng, etc)
- Green's function techniques

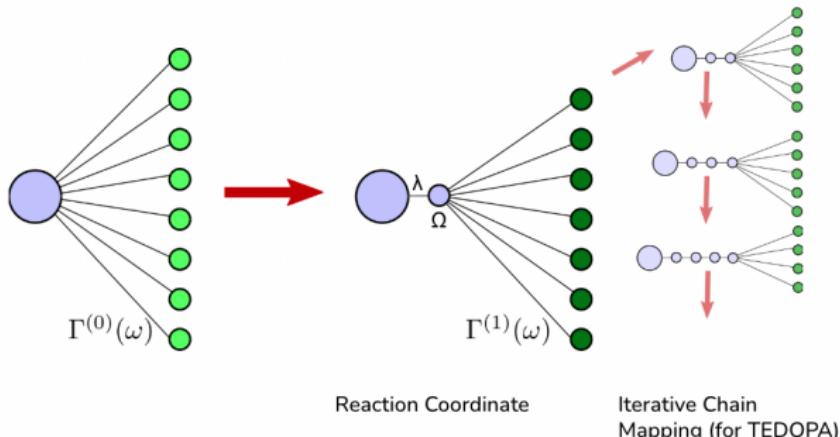
each is applicable in very particular circumstances.

Question 2:

- Inexact analytical:
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 - Green's function techniques
- each is applicable in very particular circumstances.
- the reaction-coordinate quantum master equation method is in between: a *semi-analytical* method.

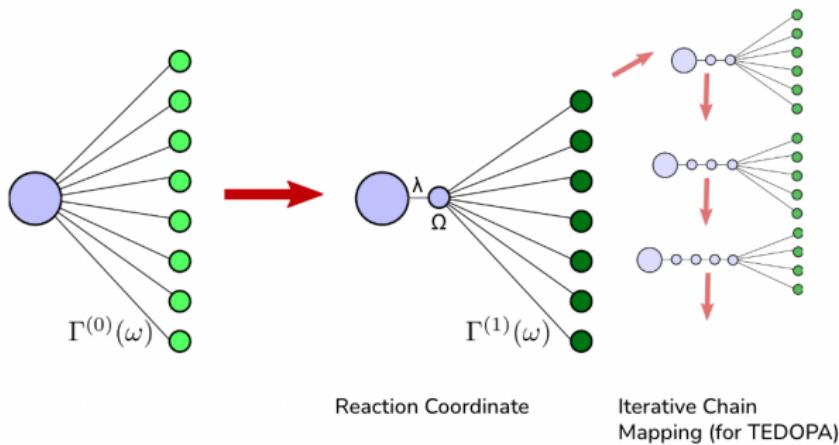
Reaction Coordinate Mapping: Primer (Chain Mapping)

Recall that the quantum system is coupled to many harmonic oscillators...



Reaction Coordinate Mapping: Primer (Chain Mapping)

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- A couple words on TEDOPA... (a) numerically exact mapping through orthogonal polynomials, (b) infinitely long chain \rightarrow truncated chain (bounded by Lieb-Robinson technique) + truncated harmonic manifold, (c) evolved with DMRG or TEBD, essentially evolving the whole chain, must Trotterize.

Reaction Coordinate Mapping: Details

$$\hat{H} = \hat{H}_s + \sum_k \nu_k \left(\hat{c}_k^\dagger + \hat{S} \frac{f_k}{\nu_k} \right) \left(\hat{c}_k + \hat{S} \frac{f_k}{\nu_k} \right) \quad (17)$$



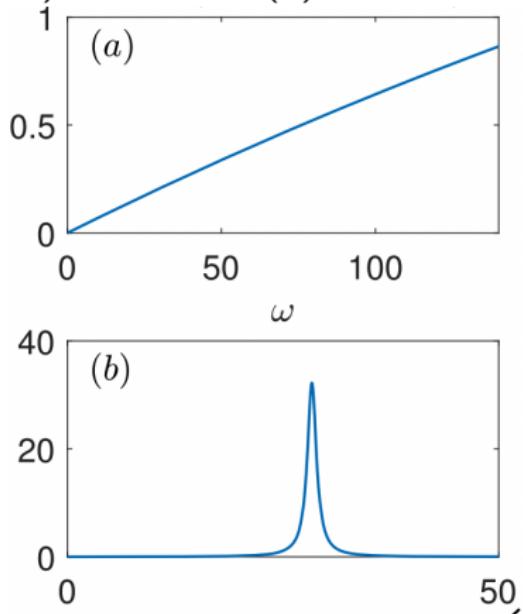
$$\begin{aligned} \hat{H} &= \hat{H}_s + \Omega \left(\hat{a}^\dagger + \frac{\lambda}{\Omega} \hat{S} \right) \left(\hat{a} + \frac{\lambda}{\Omega} \hat{S} \right) \\ &\quad + \sum_k \omega_k \left(\hat{b}_k^\dagger + (\hat{a} + \hat{a}^\dagger) \frac{f_k}{\omega_k} \right) \left(\hat{b}_k + (\hat{a} + \hat{a}^\dagger) \frac{f_k}{\omega_k} \right) \end{aligned} \quad (18)$$

where $\lambda(\hat{a}^\dagger + \hat{a}) = \sum_k f_k(\hat{c}^\dagger + \hat{c})$. Note that

- The system Hamiltonian (Red) expands
- The coupling is redrawn, from initial system → bath to extracted mode → residual bath

Reaction Coordinate Mapping: Details

Also, $J(\omega) \rightarrow J_{RC}(\omega)$ (quite technical, see⁵). A fair simplification is from a Brownian (peaked) J about Ω (b) \rightarrow an Ohmic (linear) J_{RC} (a)



⁵Nicholas Anto-Sztrikacs and Dvira Segal, 2021 NJP

Some remarks on the RCQME

- After the mapping, we perform BMR-QME, as the residual system-bath coupling parameter is small.
- A truncation is performed on the reaction mode, so that the extended system Hamiltonian is finite.
 - Hence, RCQME is not intended for high-temperature dynamics.
 - The extended Hamiltonian scales as
$$(\#_{\text{system levels}})(\#_{\text{extracted manifold}})^{\#_{\text{extracted bath}}}$$
. Numerical complexity \propto power 4th of extended Hamiltonian dimension to construct Redfield tensor.
- A partial trace over the reaction modes is then taken to revert back to the (original) system basis.
- Can use existing toolbox developed for BMR-QME or Lindblad QME.

Applications of the RCQME (from the Segal group)

- Mostly numerical:
 - Non-equilibrium spin-boson at strong coupling⁶
 - **Quantum absorption refrigerator at strong coupling**⁷
 - Markovian dynamics⁸
- Analytical:
 - **Transport beyond second order**⁹
 - Generalized effective hamiltonian theory¹⁰

⁶Nicholas Anto-Sztrikacs and Dvira Segal, 2021 NJP

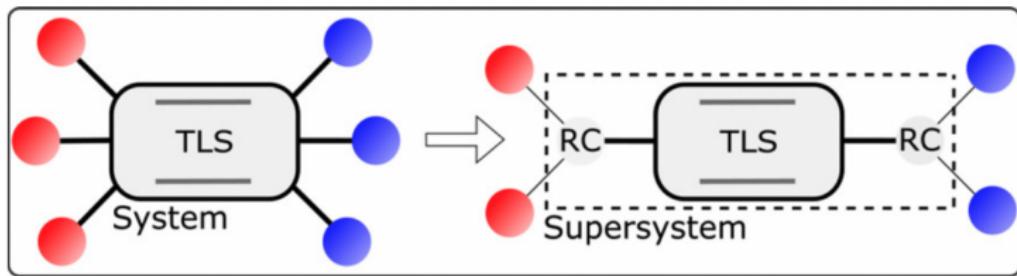
⁷FI*, NAS*, and DS, 2022 PRE

⁸NAS and DS, 2021 PRA

⁹NAS, FI, and DS, 2022 JCP

¹⁰NAS, Ahsan Nazir, and DS, 2023 PRX Quantum

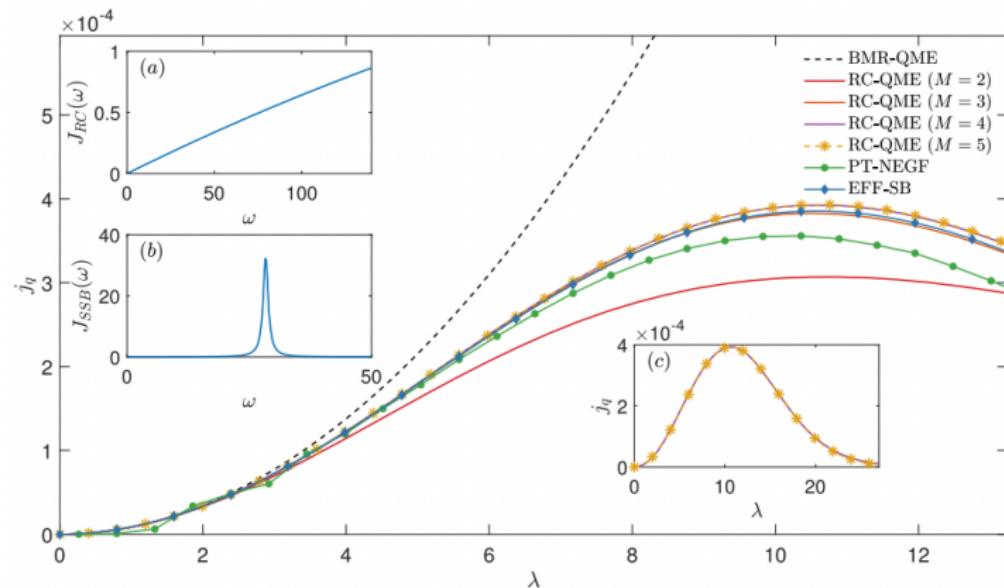
Non-equilibrium spin-boson at strong coupling¹¹



We'd like to know $j_{q,i} = \text{Tr}\left\{ D_i(\rho_{ES}) \hat{H}_{ES} \right\}$ (i.e., how conductive the qubit is) at steady state

¹¹Nicholas Anto-Sztrikacs and Dvira Segal, 2021 NJP

Non-equilibrium spin-boson at strong coupling¹²



- RC-QME captures a signature of strong-coupling transport, turnover.
- RC-QME agrees with numerically intensive methods, PT-NEGF.

¹²Nicholas Anto-Sztrikacs and Dvira Segal, 2021 NJP

Signature of strong coupling: energy renormalization

Energy renormalization causes turnover behaviour. At low temperature...

- Squeeze slightly \Rightarrow low cost to excite effective qubit \Rightarrow higher current
- Squeeze too much \Rightarrow each photon carries little energy \Rightarrow lower current

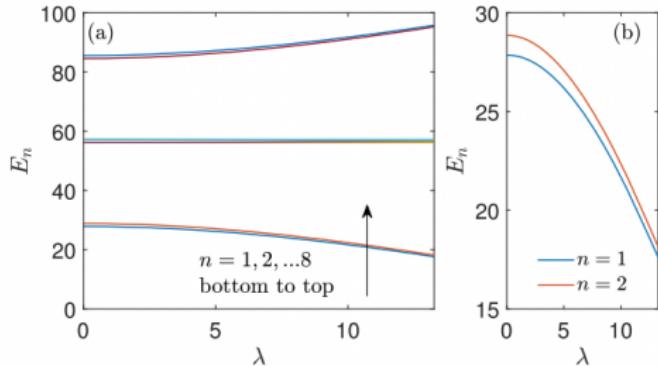
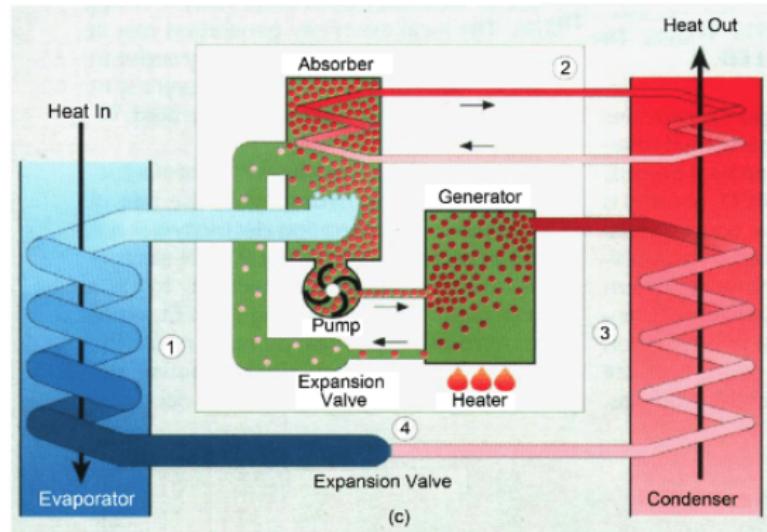


Figure 2. (a) Eigenenergies of $H_{\text{ES}}^{M=2}$ with $\Delta = 1$, $\varepsilon = 0$, $\Omega = 28\Delta$ [65]. (b) Focus on the lowest two eigenvalues, which form an effective spin Hamiltonian.

Quantum Absorption Refrigerator at strong coupling¹³

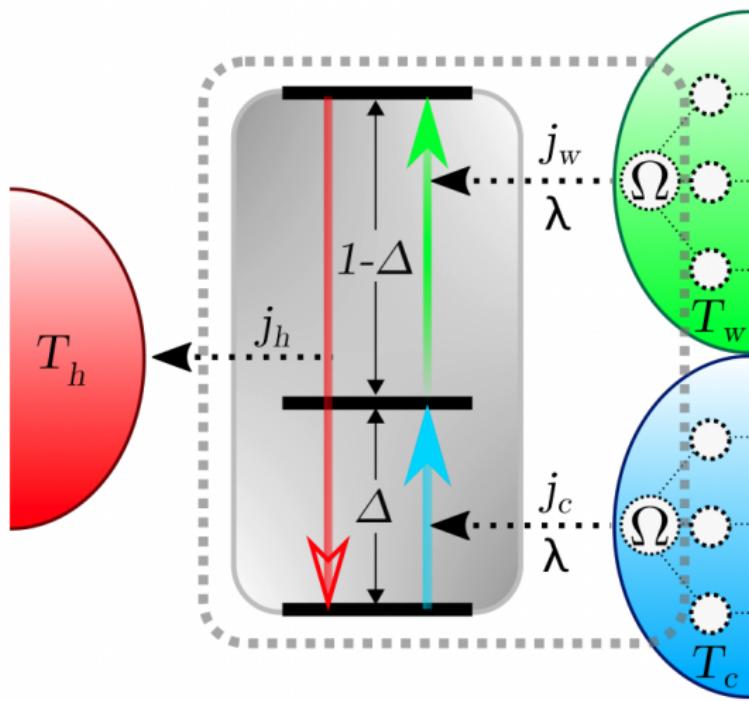
an Absorption Refrigerator takes in heat from T_c and dumps it to T_h using work from T_w ($T_w > T_h > T_c$).



¹³FI*, NAS*, and DS, 2022 PRE

Quantum Absorption Refrigerator at strong coupling¹⁴

This refrigerator is therefore quantummable.



Quantum Absorption Refrigerator at strong coupling¹⁵

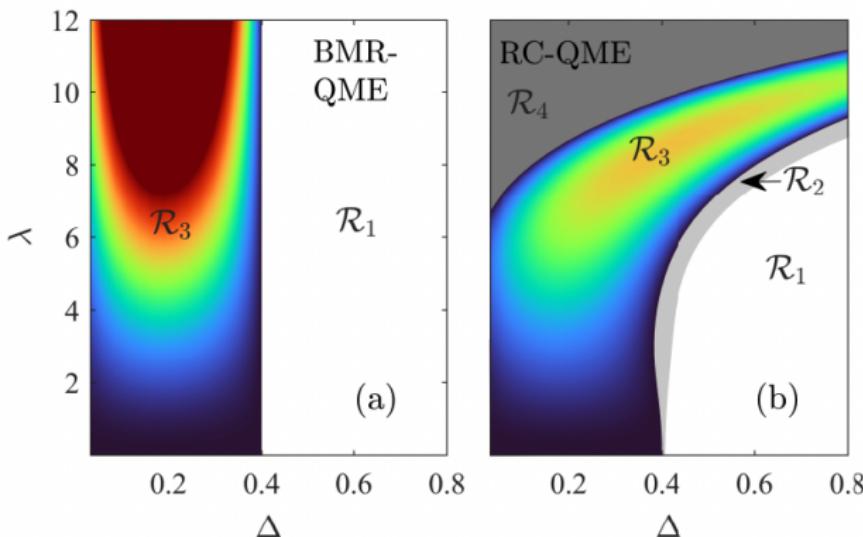
In the tight-coupling limit (i.e., one quanta in one quanta out) one can prove

$$\frac{\epsilon_2 - \epsilon_1}{\epsilon_3 - \epsilon_1} \leq \frac{\beta_h - \beta_w}{\beta_c - \beta_w} \Leftrightarrow \text{cooling} \quad (19)$$

also, from BMR-QME, higher λ leads to better cooling.

Quantum Absorption Refrigerator at strong coupling¹⁶

With strong coupling,

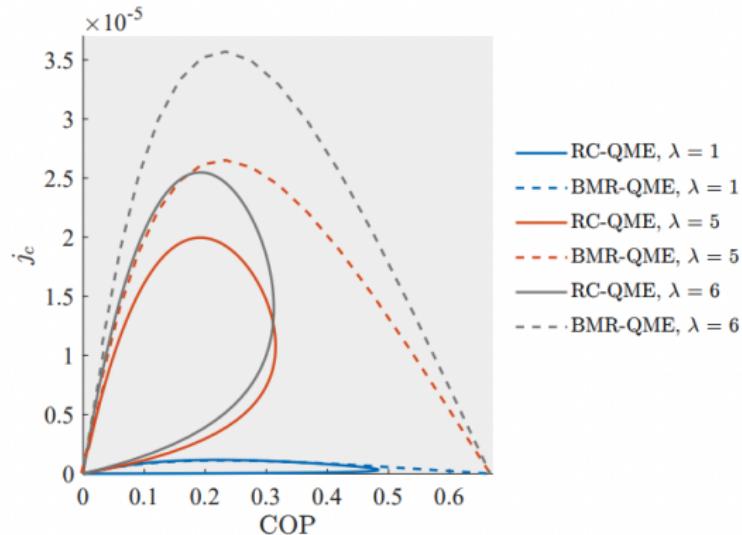


- Reshaping of cooling region, \mathcal{R}_3 (Renormalization)
- Emergence of new transport pathways , \mathcal{R}_2 (Bath-bath pathway)

¹⁶FI*, NAS*, and DS, 2022 PRE

Quantum Absorption Refrigerator at strong coupling¹⁷

And therefore we'll never hit Carnot's efficiency,



¹⁷FI*, NAS*, and DS, 2022 PRE

Quantum transport beyond second order

Recall in the derivation of BMR-QME, we cut the Dyson series to second order. Some nontrivial effects can arise **even** at weak coupling, if we had kept on going.

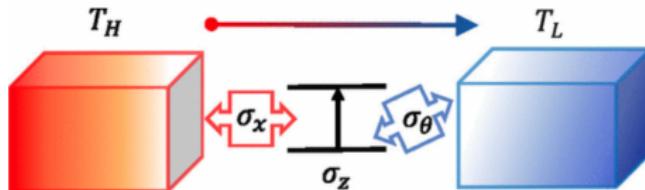
One example is the $\sigma_x - \sigma_z$ type transport reported in Ref.¹⁸

¹⁸Jianshu Cao et al., JCP 2020

Quantum transport beyond second order

Consider the generalized non-equilibrium spin-boson (NESB) model,

$$\begin{aligned}\hat{H}_{SB} = & \frac{\Delta}{2} \hat{\sigma}_z + \hat{\sigma}_x \sum_k f_{k,L} (\hat{c}_{k,L}^\dagger + \hat{c}_{k,L}) \\ & + \underbrace{\hat{\sigma}_\theta}_{\hat{\sigma}_z \cos(\theta) + \hat{\sigma}_x \sin(\theta)} \sum_k f_{k,R} (\hat{c}_{k,R}^\dagger + \hat{c}_{k,R}) \\ & + \sum_{k,\alpha \in \{R,L\}} \nu_{k,\alpha} \hat{c}_{k,\alpha}^\dagger \hat{c}_{k,\alpha}.\end{aligned}\quad (20)$$



Quantum transport beyond second order

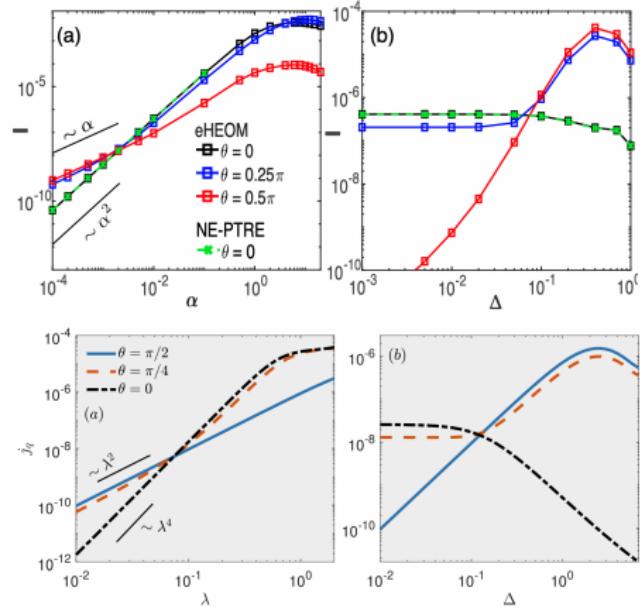
It could be shown that the heat current at steady state takes

$$\begin{aligned} j_q &\equiv -\langle \dot{\hat{H}}_{B,L} \rangle = -i\langle [\hat{H}, \hat{H}_{B,L}] \rangle, \\ &= -i\lambda_L^2 \langle [\hat{H}_S, \hat{V}_L] \rangle - i\lambda_L^2 \lambda_R^2 \langle [\hat{V}_R, \hat{V}_L] \rangle. \end{aligned} \quad (21)$$

the first term is captured by second-order BMR-QME, but the second term is not. The latter is an **interbath** transport pathway, which also appeared as leakage for QAR at strong coupling.

Quantum transport beyond second order

Numerically intensive HEOM and NE-PTRE captures $j_q \propto \lambda^4$ current¹⁹,
but RC-QME captures them just as well²⁰.



¹⁹ Jianshu Cao et al., JCP 2020

²⁰ NAS, FI, and DS, JCP 2022

Hints of analyticity with the RC-QME

The Polaron transform (the PT in NE-PTRE) is used to treat strong-coupling effects in very particular cases, modifying \hat{V} in return for dressing \hat{H}_s . Performing PT post reaction-coordinate mapping reveals interesting analytical results.

The RC-mapped Hamiltonian for Eq. (20) is

$$\begin{aligned}\hat{H}_{SB-RC} = & \frac{\Delta}{2} \hat{\sigma}_z + \Omega_L \hat{a}_L^\dagger \hat{a}_L + \Omega_R \hat{a}_R^\dagger \hat{a}_R + \lambda_L \hat{\sigma}_x (\hat{a}_L^\dagger + \hat{a}_L) \\ & + \lambda_R \hat{\sigma}_\theta (\hat{a}_R^\dagger + \hat{a}_R) + \sum_{k,\alpha} \frac{g_{k,\alpha}^2}{\omega_{k,\alpha}} (\hat{a}_\alpha^\dagger + \hat{a}_\alpha)^2 \\ & + \sum_\alpha (\hat{a}_\alpha^\dagger + \hat{a}_\alpha) \sum_k g_{k,\alpha} (\hat{b}_{k,\alpha}^\dagger + \hat{b}_{k,\alpha}) + \sum_{k,\alpha} \omega_{k,\alpha} \hat{b}_{k,\alpha}^\dagger \hat{b}_{k,\alpha}.\end{aligned}\tag{22}$$

Transform that Hamiltonian, $\hat{H}_{SB-RC} = \hat{U}_P \hat{H}_{SB-RC} \hat{U}_P^\dagger$, to the left reservoir with $\hat{U}_P^L = e^{\frac{\lambda_L}{\Omega_L} \hat{\sigma}_x (\hat{a}_L^\dagger - \hat{a}_L)}$. This results to

At low temperatures, $\Delta \rightarrow \Delta e^{-\frac{\lambda^2}{2\Omega^2}}$

$$\begin{aligned}\hat{H}_{SB-RC} = & \boxed{\frac{\Delta}{4} \left[(\hat{\sigma}_z - i\hat{\sigma}_y) e^{\frac{\lambda_L}{\Omega_L} (\hat{a}_L^\dagger - \hat{a}_L)} + (\hat{\sigma}_z + i\hat{\sigma}_y) e^{-\frac{\lambda_L}{\Omega_L} (\hat{a}_L^\dagger - \hat{a}_L)} \right]} + \Omega_R \hat{a}_R^\dagger \hat{a}_R + \Omega_L \hat{a}_L^\dagger \hat{a}_L \\ & + \lambda_R \sin \theta (\hat{a}_R^\dagger + \hat{a}_R) \hat{\sigma}_x + \lambda_R \cos \theta (\hat{a}_R^\dagger + \hat{a}_R) \frac{1}{2} \left[(\hat{\sigma}_z - i\hat{\sigma}_y) e^{\frac{\lambda_L}{\Omega_L} (\hat{a}_L^\dagger - \hat{a}_L)} + (\hat{\sigma}_z + i\hat{\sigma}_y) e^{-\frac{\lambda_L}{\Omega_L} (\hat{a}_L^\dagger - \hat{a}_L)} \right] \\ & - \frac{2\lambda_L}{\Omega_L} \hat{\sigma}_x \sum_k g_{k,L} (\hat{b}_{k,L}^\dagger + \hat{b}_{k,L}) + (\hat{a}_L^\dagger + \hat{a}_L - \frac{2\lambda_L}{\Omega_L} \hat{\sigma}_x)^2 \sum_k \frac{g_{k,L}^2}{\omega_{k,L}} + (\hat{a}_R^\dagger + \hat{a}_R)^2 \sum_k \frac{g_{k,R}^2}{\omega_{k,R}} \\ & + \sum_\alpha (\hat{a}_\alpha^\dagger + \hat{a}_\alpha) \sum_k g_{k,\alpha} (\hat{b}_{k,\alpha}^\dagger + \hat{b}_{k,\alpha}) + \sum_{k,\alpha} \omega_{k,\alpha} \hat{b}_{k,\alpha}^\dagger \hat{b}_{k,\alpha}.\end{aligned}$$

Set $\theta = \pi/2$ and perform an additional polaron transform on the right reservoir. At low temperatures and to lowest order in λ ,

$$\begin{aligned}\hat{H}_{SB-RC}^{\sigma_x-\sigma_x} &= \frac{\Delta}{2} \hat{\sigma}_z - \frac{\Delta}{2} i \hat{\sigma}_y \sum_{\alpha} \frac{\lambda_{\alpha}}{\Omega_{\alpha}} (\hat{a}_{\alpha}^{\dagger} - \hat{a}_{\alpha}) + \Omega_R \hat{a}_R^{\dagger} \hat{a}_R + \Omega_L \hat{a}_L^{\dagger} \hat{a}_L \\ &\quad + \boxed{\sum_{\alpha} (\hat{a}_{\alpha}^{\dagger} + \hat{a}_{\alpha}) \left[\hat{\sigma}_x \left(\frac{-2\lambda_{\alpha}}{\Omega_{\alpha}} \right) \sum_k \frac{g_{k,\alpha}^2}{\omega_{k,\alpha}} + \sum_k g_{k,\alpha} (\hat{b}_{k,\alpha}^{\dagger} + \hat{b}_{k,\alpha}) \right]} \\ &\quad - \sum_{\alpha} \frac{2\lambda_{\alpha}}{\Omega_{\alpha}} \hat{\sigma}_x \sum_k g_{k,\alpha} (\hat{b}_{k,\alpha}^{\dagger} + \hat{b}_{k,\alpha}) + \sum_{k,\alpha} \omega_{k,\alpha} \hat{b}_{k,\alpha}^{\dagger} \hat{b}_{k,\alpha} \\ &\quad + \sum_{\alpha} (\hat{a}_{\alpha}^{\dagger} + \hat{a}_{\alpha})^2 \sum_k \frac{g_{k,\alpha}^2}{\omega_{k,\alpha}}.\end{aligned}$$

One bath excites RC \rightarrow RC excites system via $\sigma_x \rightarrow$ the other bath.

Set $\theta = 0$,

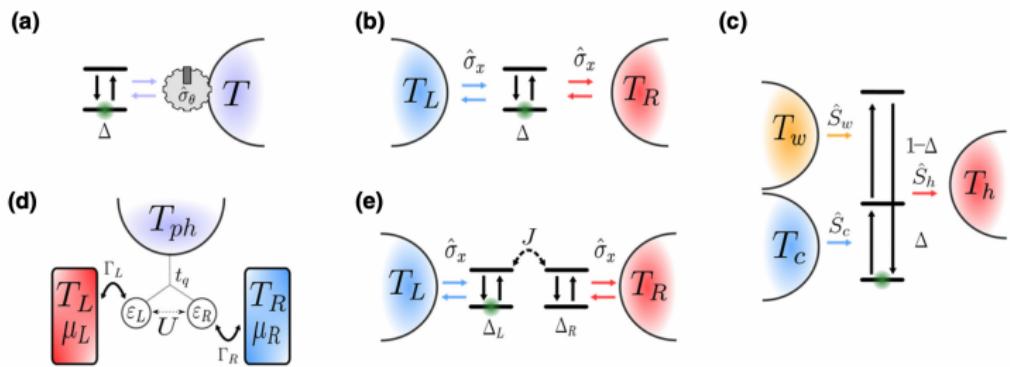
$$\begin{aligned}
 \hat{H}_{SB-RC}^{\sigma_x - \sigma_z} = & \frac{\Delta}{2} \hat{\sigma}_z - \frac{i\lambda_L \Delta}{2\Omega_L} \hat{\sigma}_y (\hat{a}_L^\dagger - \hat{a}_L) + \sum_{k,\alpha} \omega_{k,\alpha} \hat{b}_{k,\alpha}^\dagger \hat{b}_{k,\alpha} \\
 & + \Omega_R \hat{a}_R^\dagger \hat{a}_R + \Omega_L \hat{a}_L^\dagger \hat{a}_L + \lambda_R \hat{\sigma}_z (\hat{a}_R^\dagger + \hat{a}_R) \\
 & - i \frac{\lambda_R \lambda_L}{\Omega_L} (\hat{a}_R^\dagger + \hat{a}_R) \hat{\sigma}_y (\hat{a}_L^\dagger - \hat{a}_L) \\
 & - \frac{2\lambda_L}{\Omega_L} \hat{\sigma}_x \sum_k g_{k,L} (\hat{b}_{k,L}^\dagger + \hat{b}_{k,L}) + (\hat{a}_L^\dagger + \hat{a}_L - \frac{2\lambda_L}{\Omega_L} \hat{\sigma}_x)^2 \sum_k \frac{g_{k,L}^2}{\omega_{k,L}} \\
 & + (\hat{a}_R^\dagger + \hat{a}_R)^2 \sum_k \frac{g_{k,R}^2}{\omega_{k,R}} + \sum_\alpha (\hat{a}_\alpha^\dagger + \hat{a}_\alpha) \sum_k g_{k,\alpha} (\hat{b}_{k,\alpha}^\dagger + \hat{b}_{k,\alpha})
 \end{aligned}$$

Emergence of an unusual bath-bath transport pathway which scales differently as the bath-system-bath pathway.

Effective Hamiltonian Theory at strong coupling

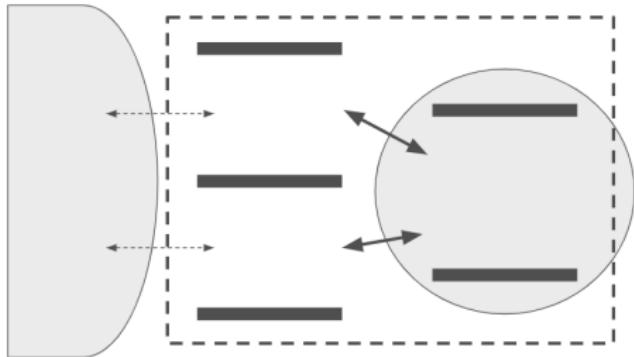
PT-RCQME was generalized by NAS, where strong coupling effects can be encoded at the Hamiltonian level simple enough to do analytical work²¹

$$\hat{H}_s^{\text{eff}}(\lambda) = \langle 0 | e^{(\lambda/\Omega)(\hat{a}^\dagger - \hat{a})\hat{S}} \hat{H}_s e^{-(\lambda/\Omega)(\hat{a}^\dagger - \hat{a})\hat{S}} | 0 \rangle.$$



²¹NAS, Ahsan Nazir, and DS, PRX Quantum 2023

Markovian dynamics with RC-QME²²



Conclusion

Reaction-coordinate master equation is an semi-analytical method to study quantum dynamics beyond Born-Markov. Signatures of strong coupling can explain complex models, for example quantum absorption refrigerators.

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