

Reaction Coordinate Master Equation for Transport Problems Beyond Born-Markov

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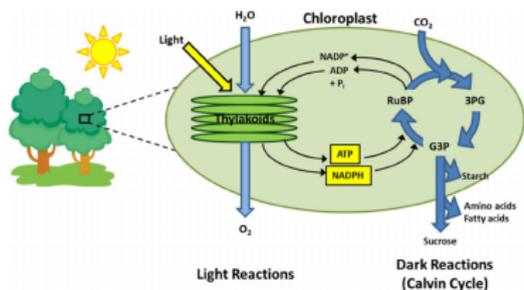
Question 1

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

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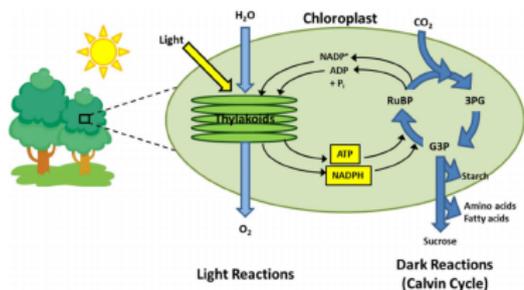
How would a **quantum** system evolve in contact with a thermal environment? ← Why is this interesting?

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



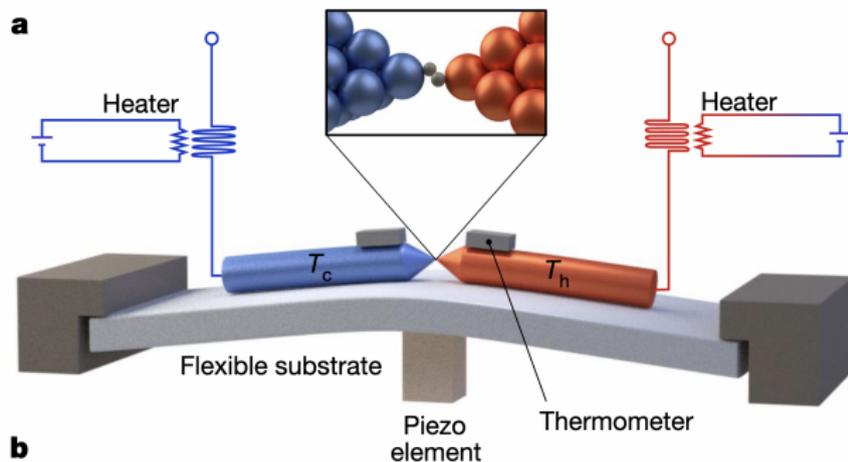
- Photosynthesis is at room temperature

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



- Photosynthesis is at room temperature
- Quantum effects in photosynthesis

Quantum 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 \rightarrow infinitely many harmonic oscillators.

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But...

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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,

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

²Breuer and Petruccione or Lidar are good references

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which Lindblad proved to take the general GKLS form²

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

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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.

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,

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

Born-Markov Redfield: Derivation Sketch

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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 " $\hat{V} \ll \hat{H}_0$ "

$$\frac{\partial \rho_I}{\partial t}(t) = -i[\hat{V}_I(t), \rho_I(t_0)] - \underbrace{\int_{t_0}^t d\tau [\hat{V}_I(t), [\hat{V}_I(\tau), \rho_I(\tau)]]}_{\text{Partial trace}} \quad (9)$$

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

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

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

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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.

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

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

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

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

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

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

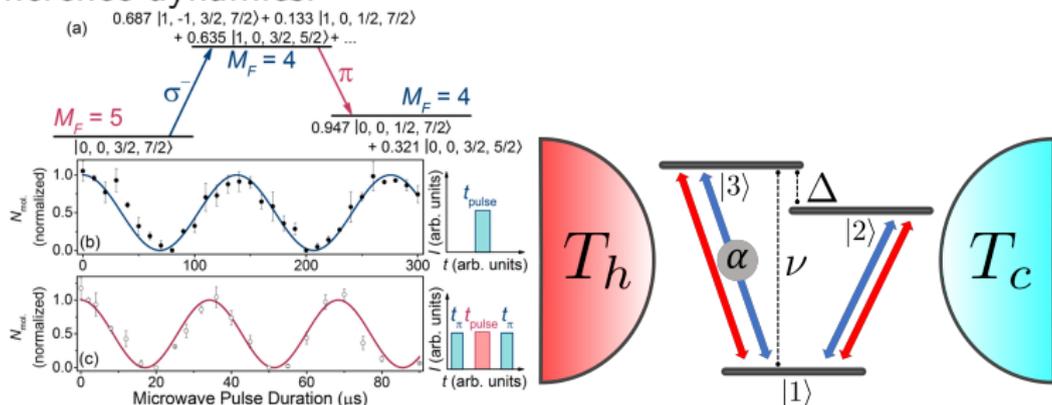
all we need to know about the environment is encoded in the spectral density $J(\omega)$.

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) \rightarrow 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.



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

⁴FI, 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:

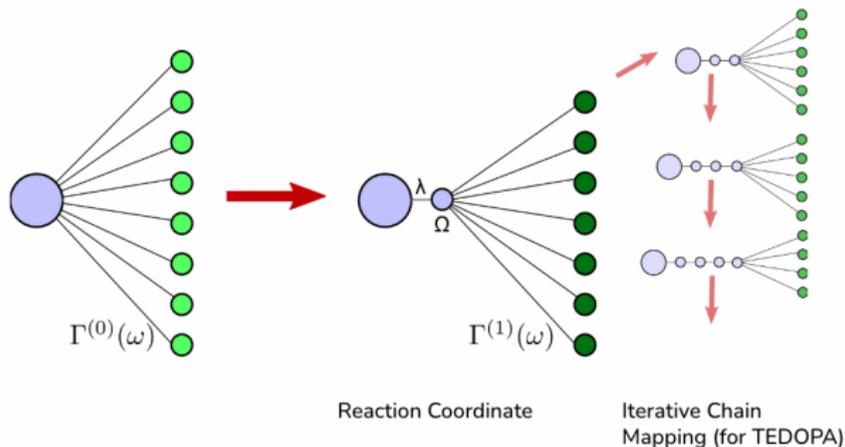
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each is applicable in very particular circumstances.

- the reaction-coordinate quantum master equation method is in between: a *semi*-analytical method.

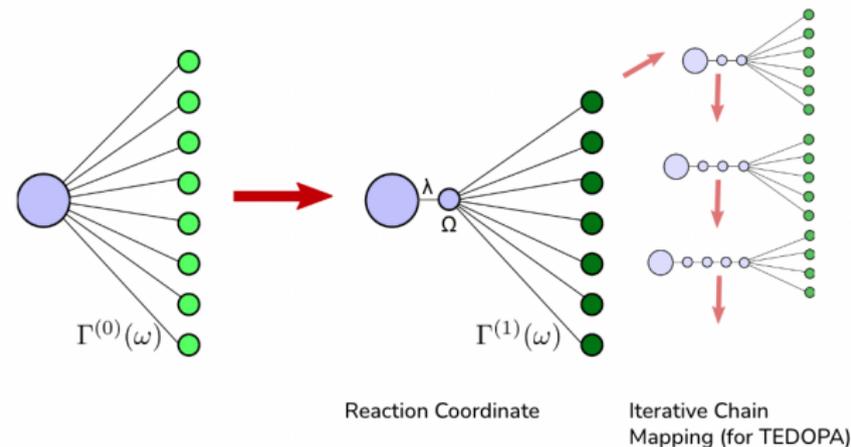
Reaction Coordinate Mapping: Primer (Chain Mapping)

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



Reaction Coordinate Mapping: Primer (Chain Mapping)

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



- 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

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



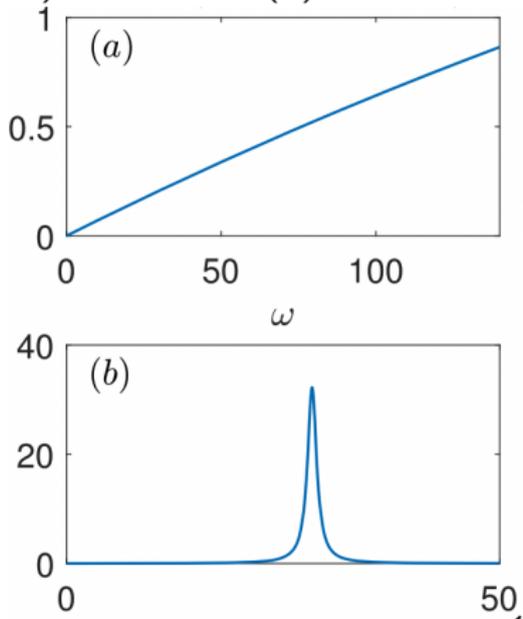
$$\begin{aligned} \hat{H} = & \hat{H}_s + \Omega \left(\hat{a}^\dagger + \frac{\lambda}{\Omega} \hat{S} \right) \left(\hat{a} + \frac{\lambda}{\Omega} \hat{S} \right) \\ & + \sum_k \omega_k \left(\hat{b}_k^\dagger + (\hat{a} + \hat{a}^\dagger) \frac{f_k}{\omega_k} \right) \left(\hat{b}_k + (\hat{a} +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

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

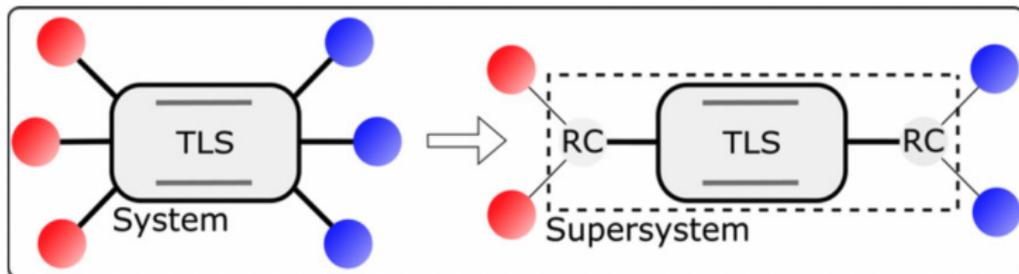
⁷FI*, NAS*, and DS, 2022 PRE

⁸NAS and DS, 2021 PRA

⁹NAS, FI, and DS, 2022 JCP

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

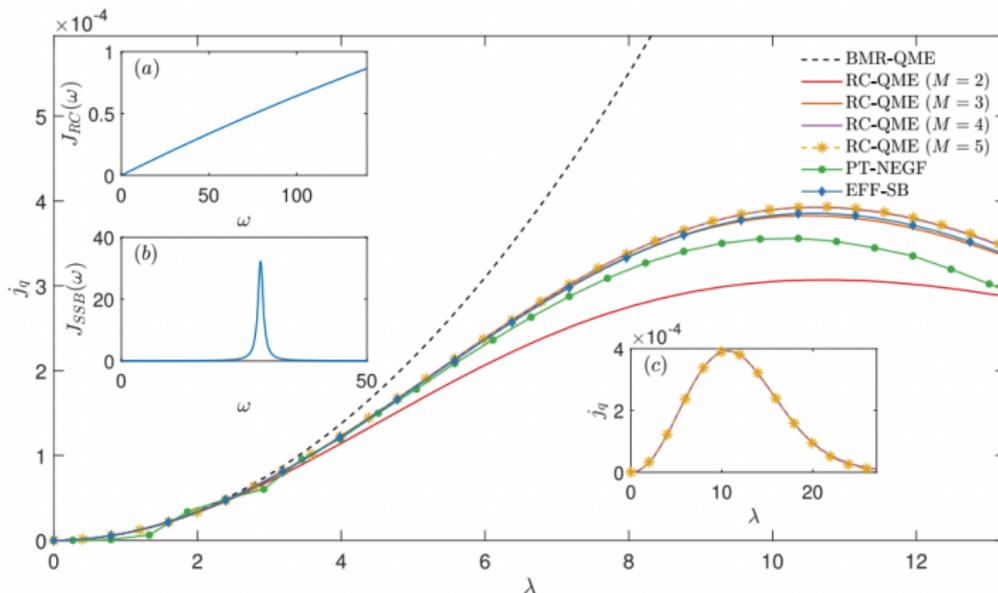
Non-equilibrium spin-boson at strong coupling¹¹



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

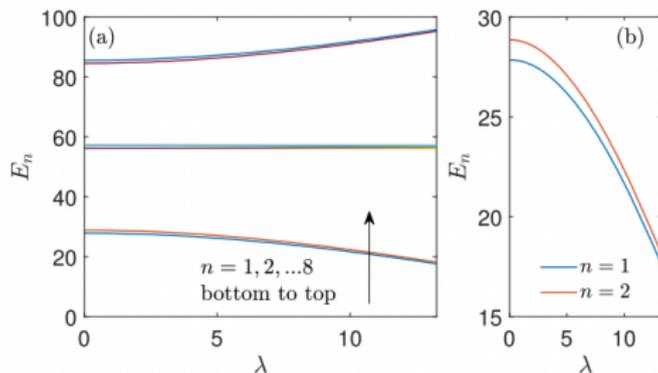
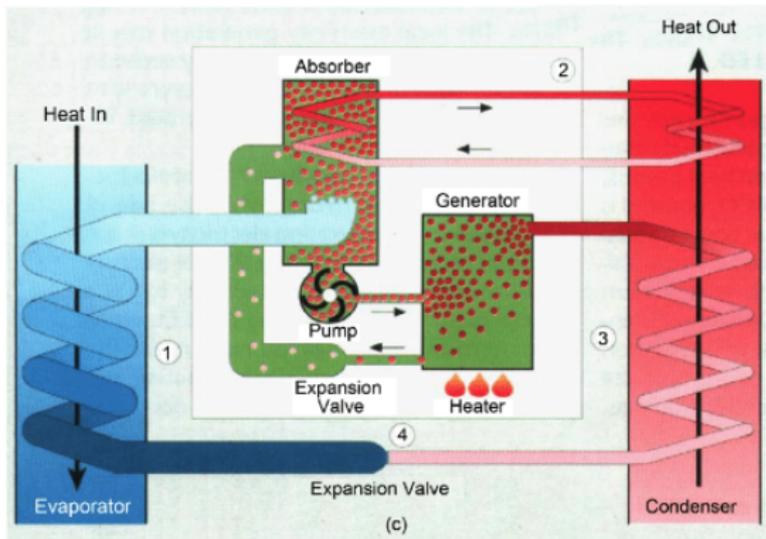


Figure 2. (a) Eigenenergies of $H_{ES}^{M=2}$ with $\Delta = 1$, $\varepsilon = 0$, $\Omega = 28\Delta$ [65]. (b) Focus on the lowest two eigenvalues, which form an effective spin Hamiltonian.

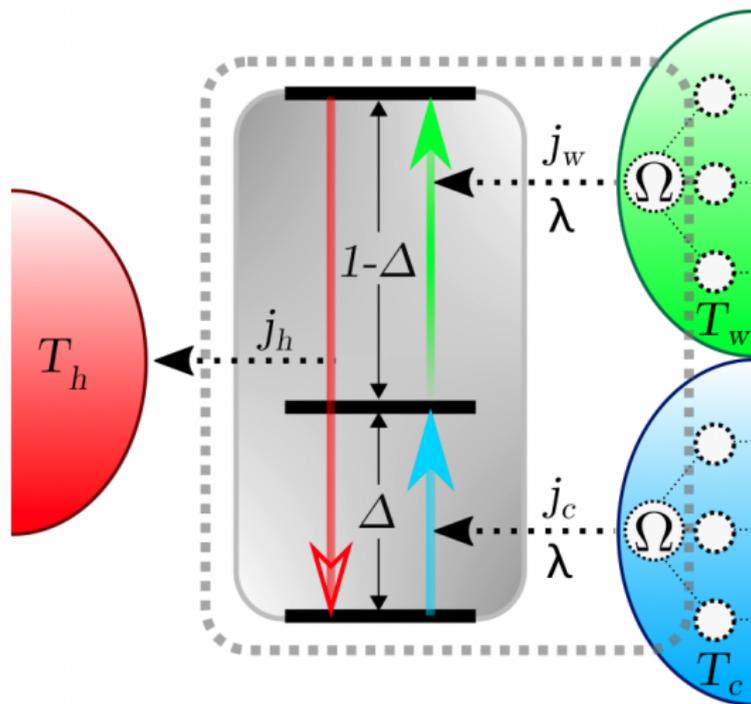
Quantum Absorption Refrigerator at strong coupling¹³

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



Quantum Absorption Refrigerator at strong coupling¹⁴

This refrigerator is therefore quantummable.



¹⁴FI*, NAS*, and DS, 2022 PRE

Quantum Absorption Refrigerator at strong coupling¹⁵

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

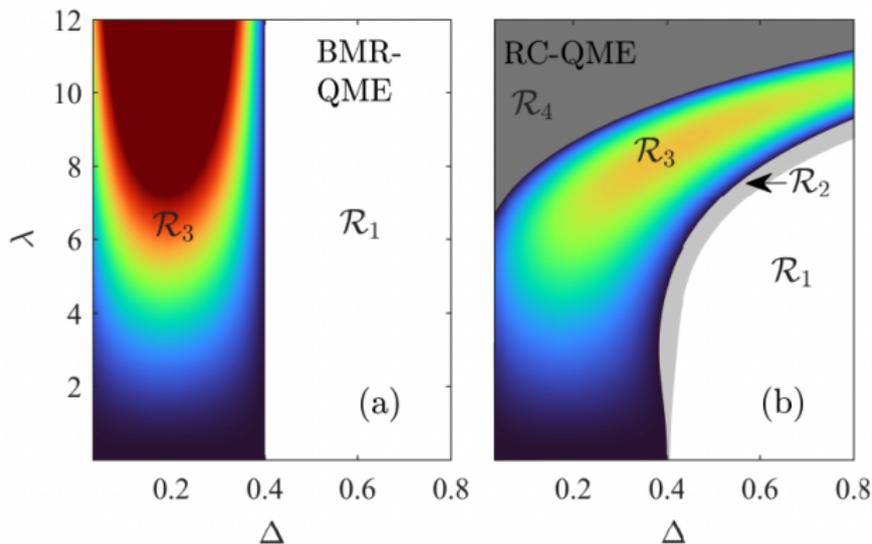
$$\frac{\epsilon_2 - \epsilon_1}{\epsilon_3 - \epsilon_1} \leq \frac{\beta_h - \beta_w}{\beta_c - \beta_w} \Leftrightarrow \text{cooling} \quad (19)$$

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

¹⁵FI*, NAS*, and DS, 2022 PRE

Quantum Absorption Refrigerator at strong coupling¹⁶

With strong coupling,

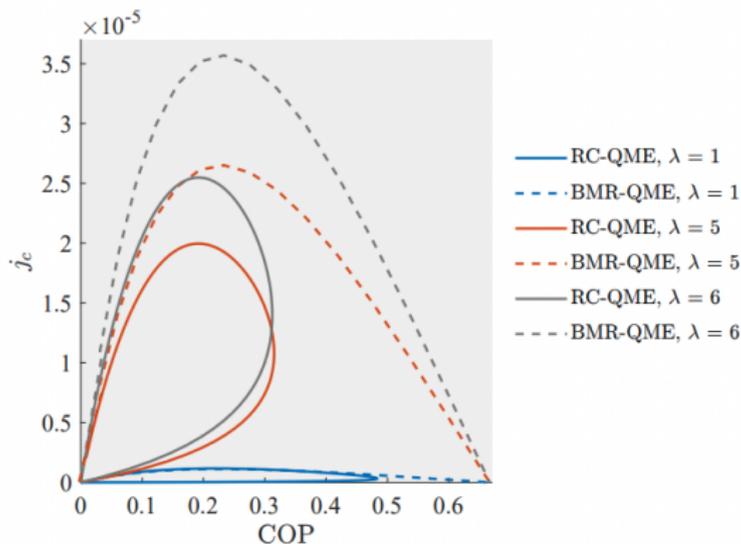


- Reshaping of cooling region, \mathcal{R}_3 (Renormalization)
- Emergence of new transport pathways, \mathcal{R}_2 (Bath-bath pathway)

¹⁶FI*, NAS*, and DS, 2022 PRE

Quantum Absorption Refrigerator at strong coupling¹⁷

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



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.

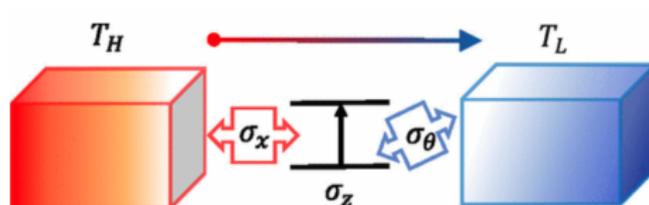
One example is the $\sigma_x - \sigma_z$ type transport reported in Ref.¹⁸

¹⁸Jianshu Cao et al., JCP 2020

Quantum transport beyond second order

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

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



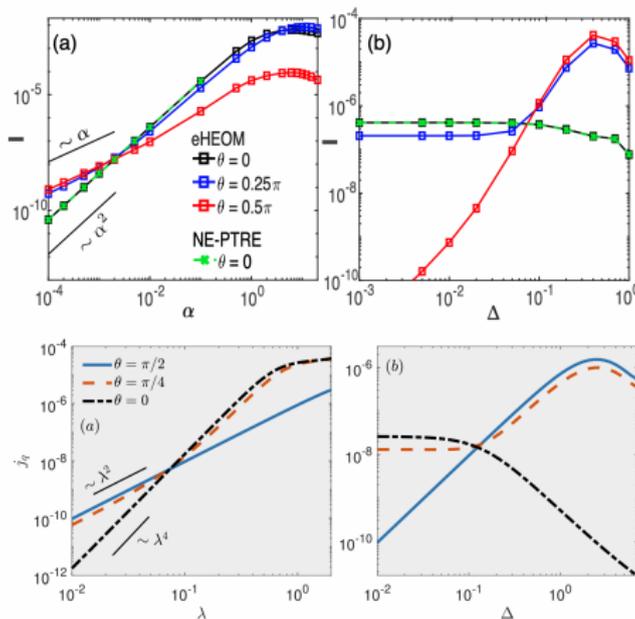
It could be shown that the heat current at steady state takes

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

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.



¹⁹Jianshu Cao et al., JCP 2020

²⁰NAS, 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, $\Delta \rightarrow \Delta e^{-\frac{\lambda^2}{2\Omega^2}}$

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

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

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

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

Set $\theta = 0$,

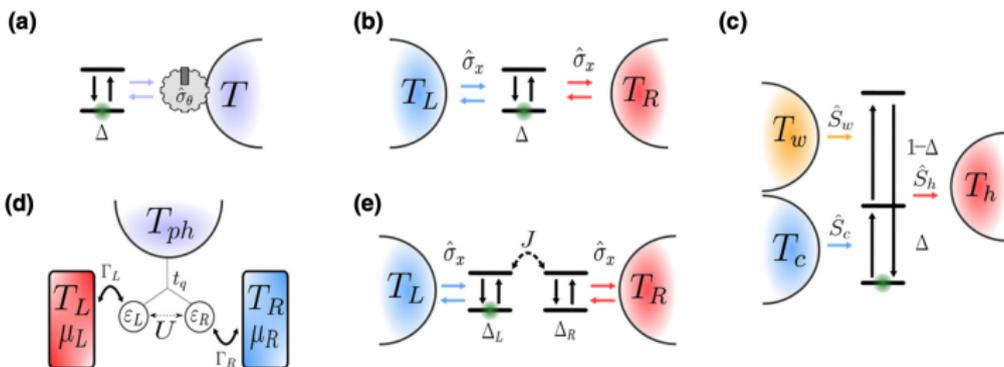
$$\begin{aligned}
 \hat{H}_{SB-RC}^{\sigma_x - \sigma_z} &= \frac{\Delta}{2} \hat{\sigma}_z - \frac{i\lambda_L \Delta}{2\Omega_L} \hat{\sigma}_y (\hat{a}_L^\dagger - \hat{a}_L) + \sum_{k,\alpha} \omega_{k,\alpha} \hat{b}_{k,\alpha}^\dagger \hat{b}_{k,\alpha} \\
 &+ \Omega_R \hat{a}_R^\dagger \hat{a}_R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

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

Effective Hamiltonian Theory at strong coupling

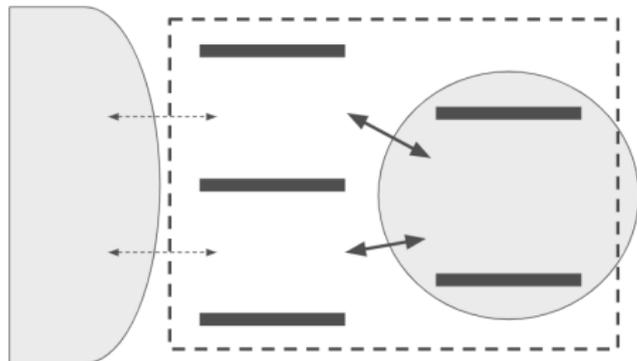
PT-RCQME was generalized by NAS, where strong coupling effects can be encoded at the Hamiltonian level simple enough to do analytical work²¹

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



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

Markovian dynamics with RC-QME²²



Conclusion

Reaction-coordinate master equation is a 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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