# Applications of the Reaction Coordinate Mapping in Quantum Thermodynamics

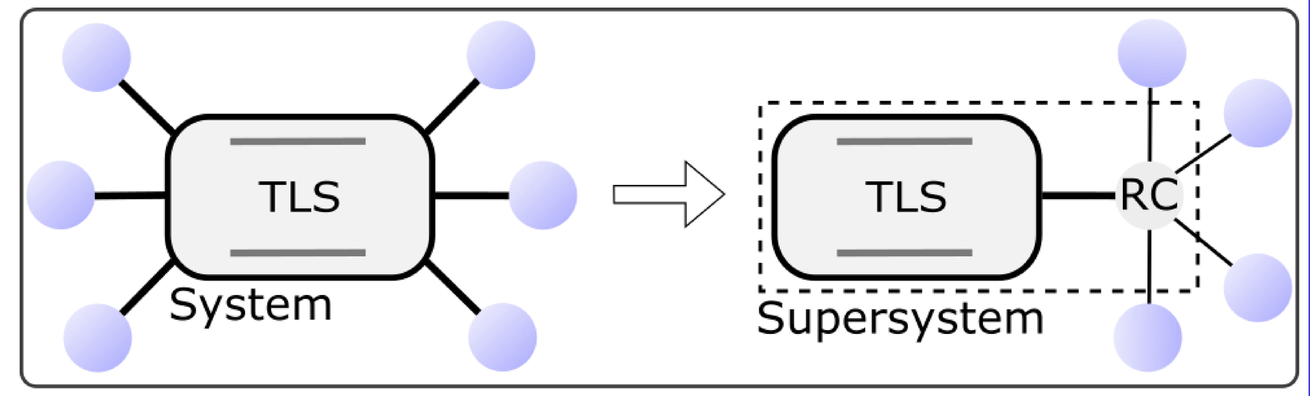
Nicholas Anto-Sztrikacs[1], Felix Ivander[2] and Dvira Segal[1,2]
Department of Physics[1], Department of Chemistry[2], University of Toronto; Toronto, Ontario, Canada

## I. Background

- Stochastic thermodynamics and quantum mechanics underpin the development of small-scale devices
- Quantum thermodynamics sets to extend the laws of thermodynamics into the quantum regime
- Strong system-reservoir coupling is a crucial aspect of thermodynamics at the nanoscale
- Standard master equation tools provide analytical insight into quantum systems, but are inaccurate in the strong coupling regime
- Numerically exact techniques offer accurate predictions, but do not provide analytical intuition
- **Research goal**: Develop a technique that is valid at strong coupling and provides accurate results and analytical insights into the role of strong coupling and apply it to develop nanoscale devices

## II. Reaction coordinate mapping

- Exact Hamiltonian mapping reshapes the system-reservoir boundary to include a collective coordinate from the environment into the system

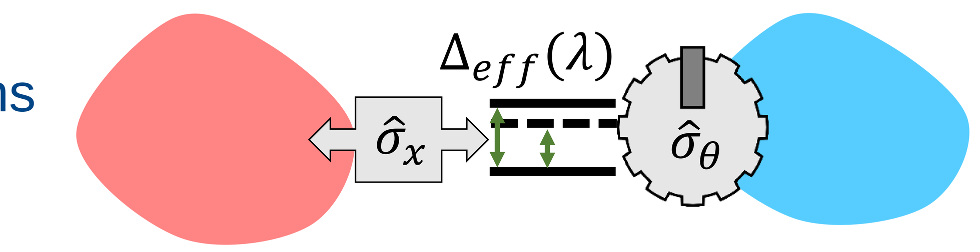



$$\hat{H} = \hat{H}_s + \hat{S}\hat{B} + \hat{H}_B \longrightarrow \hat{H}_{RC} = \hat{H}_s + \Omega\hat{a}^\dagger\hat{a} + \lambda\hat{S}(\hat{a}+\hat{a}^\dagger) + (\hat{a}+\hat{a}^\dagger)\hat{B}' + \hat{H}'_B$$

- Interaction energies $\boldsymbol{\lambda}$ are included beyond second order in perturbation theory through the inclusion of the reaction coordinate (RC) of frequency $\boldsymbol{\Omega}$
- The mapping is exact, but is most useful when the residual coupling parameter $\boldsymbol{\gamma}$ is perturbative to employ cheap master equation methods
- The method is applicable to both bosonic and fermionic systems and is general enough for applications beyond quantum thermodynamics

## III. Quantum thermal transport at strong coupling

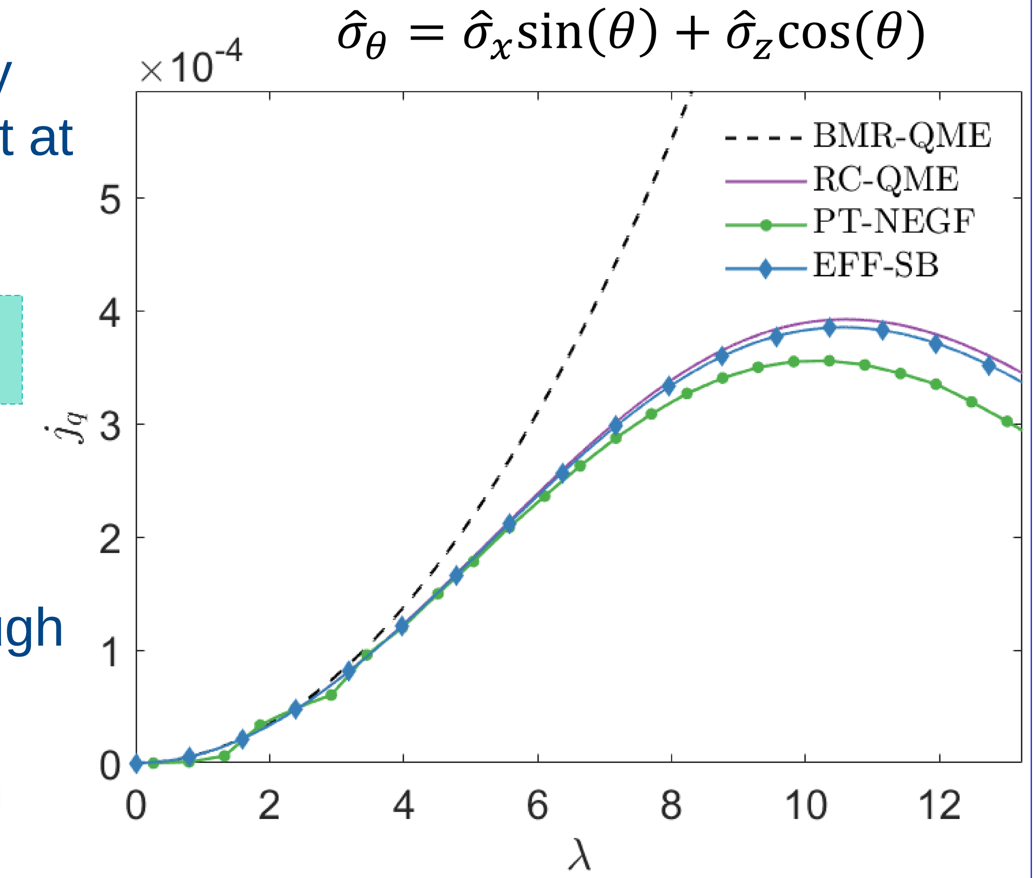
- Spin-boson model: Spin coupled to two thermal baths held at different temperatures




$$\hat{\sigma}_\theta = \hat{\sigma}_x\sin(\theta) + \hat{\sigma}_z\cos(\theta)$$

- The RC method properly captures thermal transport at strong coupling

$$\Delta_{eff}(\lambda) = \Delta e^{-2(\lambda/\Omega)^2}$$

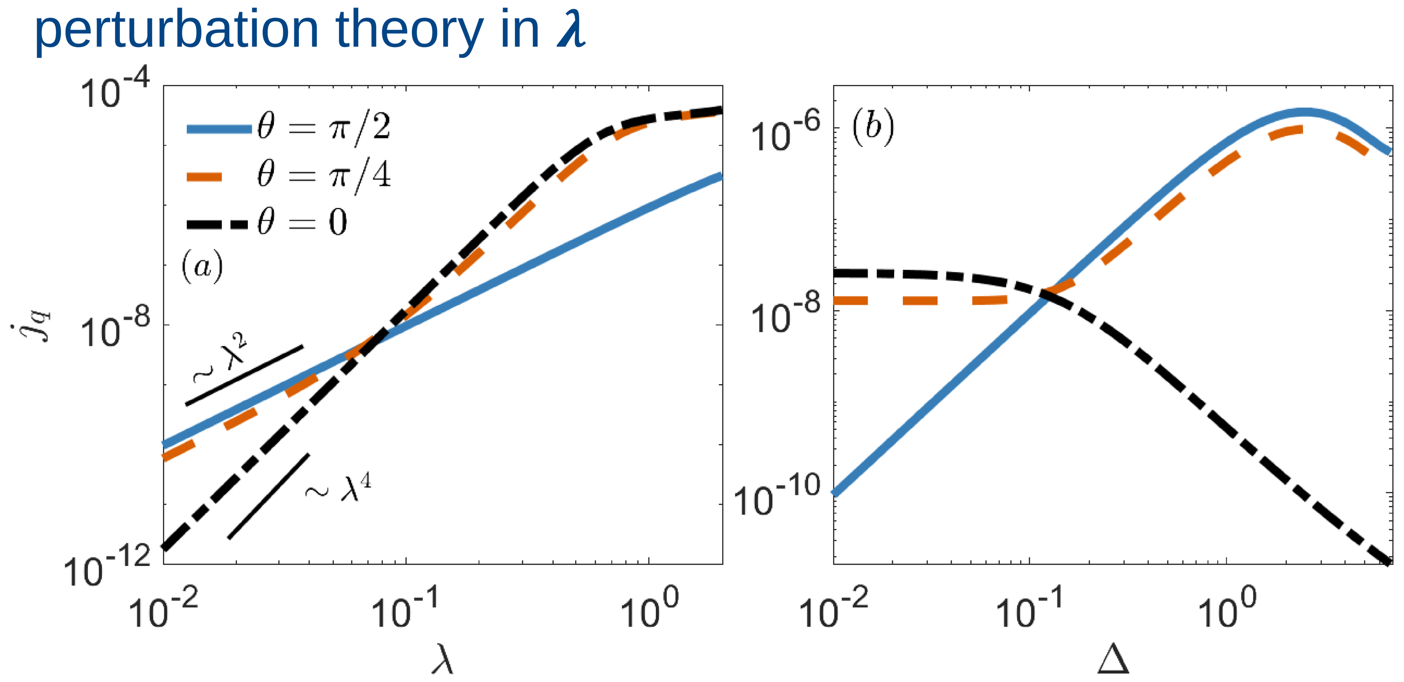



- Strong coupling **suppresses** the spin splitting, understood through an effective model
- An analytical expression for the thermal current at strong coupling emerges

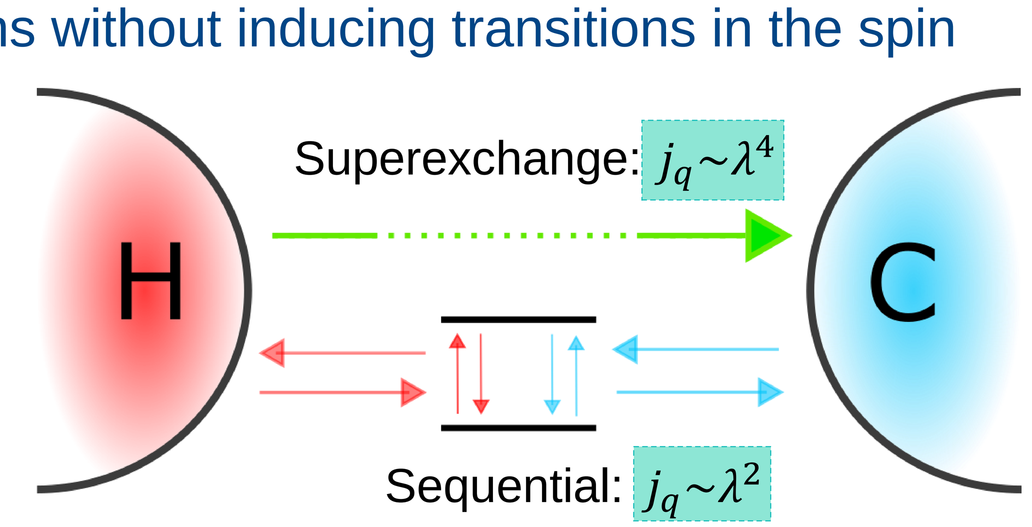
$$j_q \sim \gamma\lambda^2|\Delta_{eff}(\lambda)|^2$$

## IV. Beyond second order effects in transport

- The RC method predicts transport pathways in the spin-boson model which are beyond second order in perturbation theory in $\boldsymbol{\lambda}$




- Sequential current: mediated by transitions in the spin
- Superexchange current: exchange of quanta between baths without inducing transitions in the spin

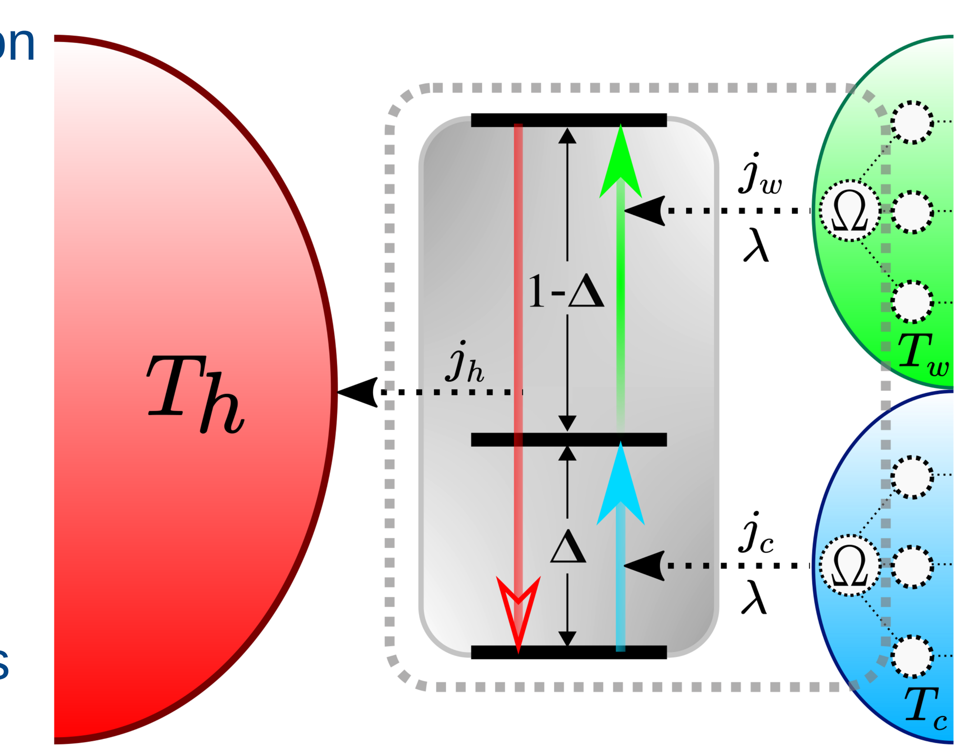



**Contact**: nicholas.antosztrikacs@mail.utoronto.ca

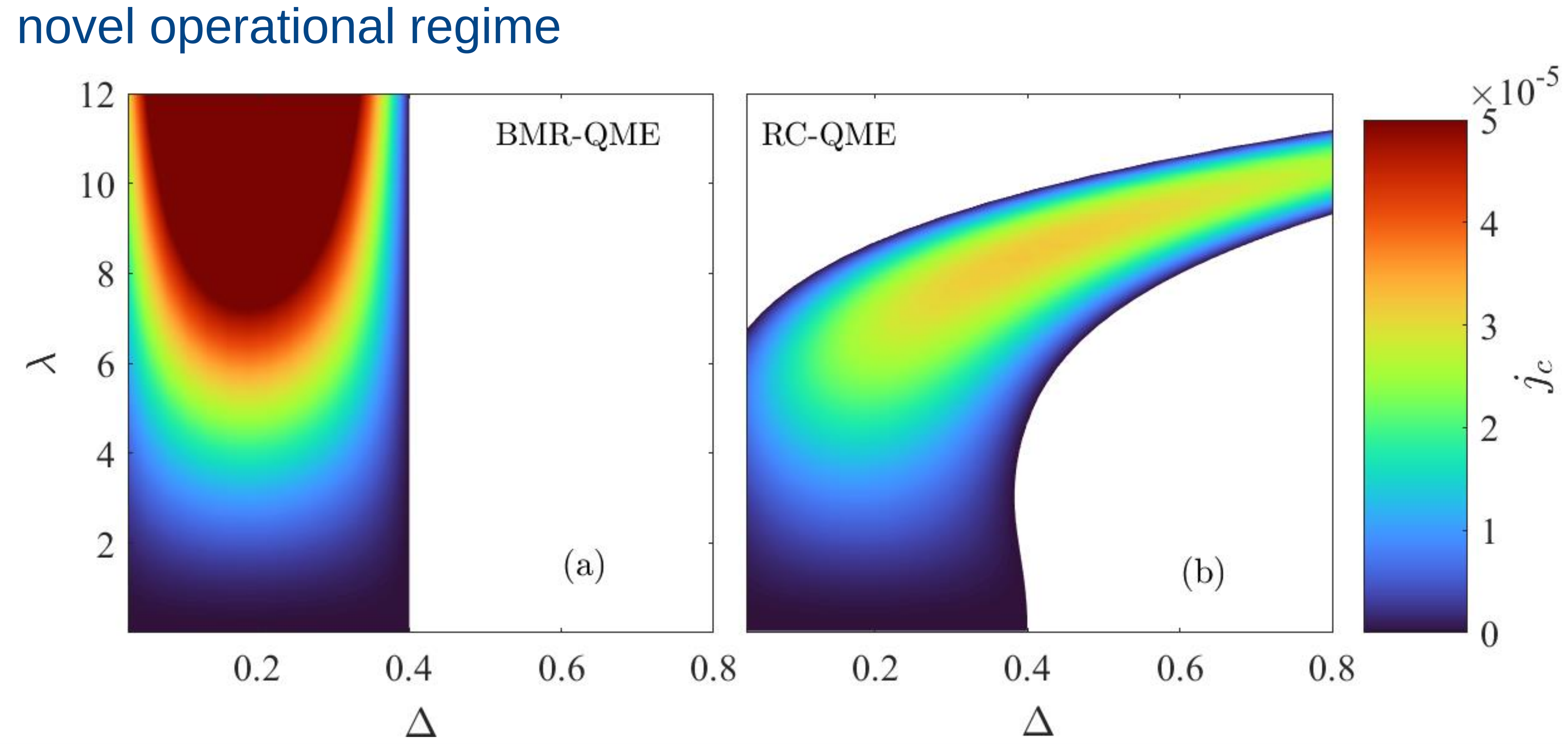
**References**:
**Anto-Sztrikacs N** and Segal D 2021 *New Journal of Physics* **23** 063036
**Anto-Sztrikacs N** and Segal D 2021 *Phys. Rev. A* **104** 052617
Ivander F*, **Anto-Sztrikacs N*** and Segal D 2022 *Phys. Rev. E* **105** 034112
**Anto-Sztrikacs N**, Ivander F and Segal D 2022 *J. Chem. Phys.* **156** 214107

## V. Quantum absorption refrigerator at strong coupling

- 3-level system, each transition coupled to separate baths at temperatures $T_c < T_h < T_w$
- A work reservoir extracts energy from a cold bath and releases it into the hot bath
- Cooling is guaranteed if the cooling condition is met
- Strong coupling renormalizes the energy levels of the QAR with $\boldsymbol{\lambda}$
- The cooling condition is **shifted** at strong coupling, offering a novel operational regime

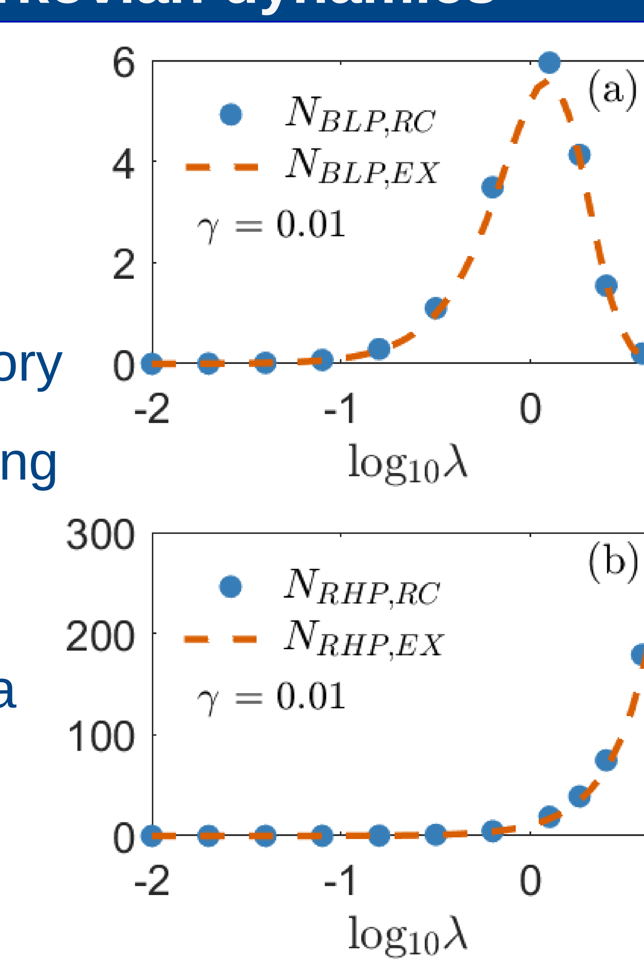



$$\frac{\Delta_{eff}(\lambda)}{1-\Delta_{eff}(\lambda)} \leq \frac{T_c(T_w - T_h)}{T_h(T_w - T_c)}$$




## VI. Characterizing non-Markovian dynamics

- Pure dephasing model: Spin-boson model with a single bosonic reservoir suffering only decoherence dynamics
- Non-Markovianity is linked to strong coupling in open quantum systems theory
- The model is exactly solvable, providing a useful benchmark for non-Markovian dynamics using the RC method
- Non-Markovianity is quantified using a distinguishability criterion between quantum states (BLP) and a characterization of the divisibility of the quantum map (RHP)




## VII. Summary

- Strong coupling effects are crucial for a correct thermodynamic description in the quantum regime
- Such strong coupling phenomena may be harnessed as a resource in the development of new nanoscale devices
- The reaction coordinate method is a versatile and powerful tool applicable in quantum thermodynamics offering accurate predictions and novel analytical insights through the lens of parameter renormalization