Quantum Coherence between Q-bits and Thermal Environments: Non-Markovian Approach.

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University of Georgia, May 18, 2017

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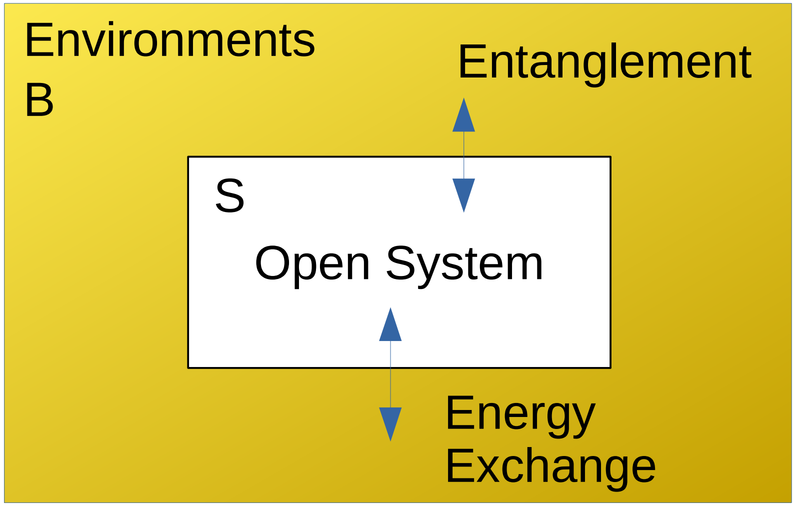
Systems in Thermal Environments



Standard Thermodynamics:

Weak Coupling between System (S) and Environment (B)

- Usually, it is strong for small systems.
- Even if it is weak, Entanglement can be formed.

Open Quantum Systems: Exact Scenario

Hamiltonian: $$H_{\mathrm{SB}} = H_{\mathrm{S}} + H_{\mathrm{B}} + V_{\mathrm{SB}}$$

Unitary Evolution
Of the Total System $$i\frac{\partial \rho_{\mathrm{SB}}}{\partial t} = [H_{\mathrm{SB}}, \rho_{\mathrm{SB}}]$$

State of the System $$\rho_{\mathrm{S}}(t) = \mathrm{tr}_{\mathrm{B}}[\rho_{\mathrm{SB}}(t)]$$

S: System, B: Thermal Bath, S+B: Isolated System

- Practically Impossible
- Need an equation of motion for $\rho_{\mathrm{S}}(t)$

Open Quantum Systems: Born-Markovian Approximation

Weak Coupling between S and B: Born Approximation
Short correlation time for B: Markovian Approximation

$$\frac{\partial \rho_{\mathrm{S}}}{\partial t} = -i\left[\tilde{H}_{\mathrm{S}}, \rho_{\mathrm{S}}\right] + D[\rho_{\mathrm{S}}]$$

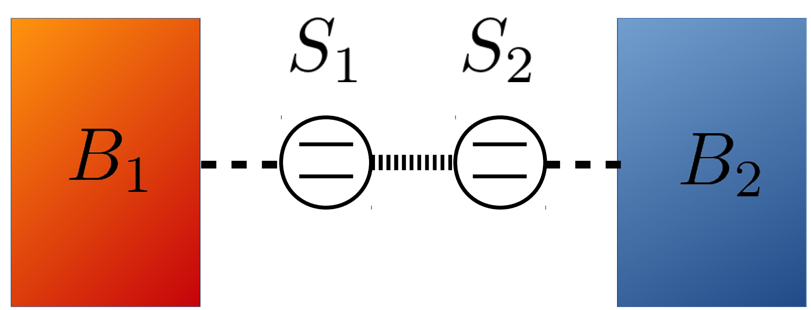
Dissipator

Quantum Master Equation

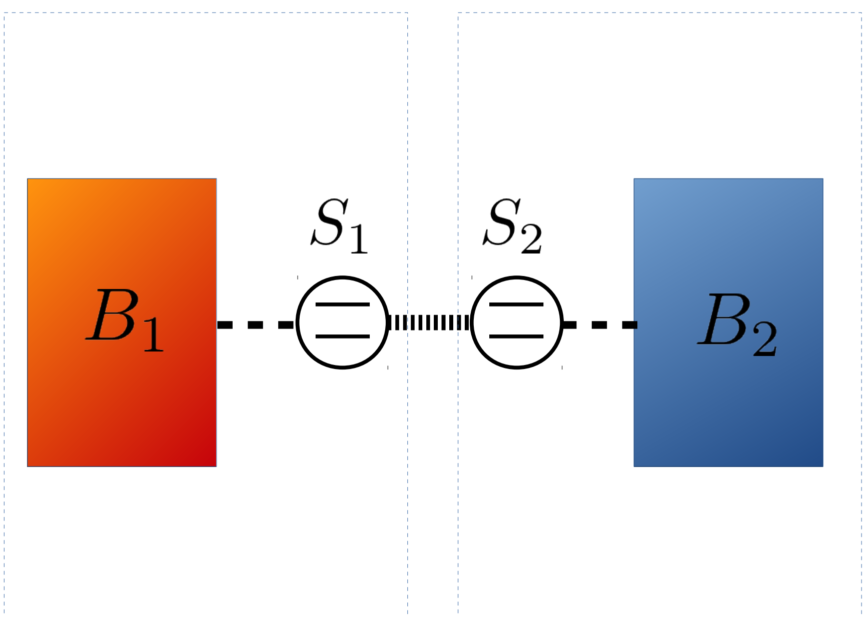
In energy eigenbasis,

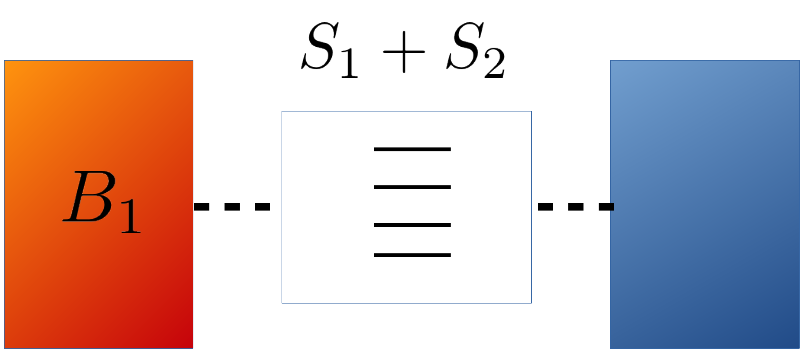
- Off-diagonal element vanishes very quickly (Decoherence)
- The transition between eigenstates is incoherent.
- No entanglement between S and B

Composite Systems

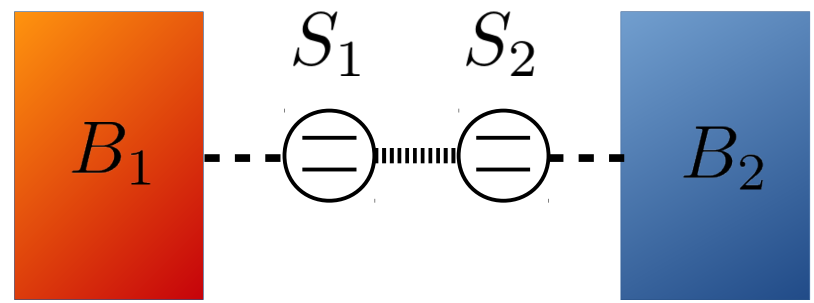


Four time scales
1)system relaxation time
2)memory in environment
3)S-B coupling strength
4)Internal coupling strength





Specific Model



Coupled Q-bits

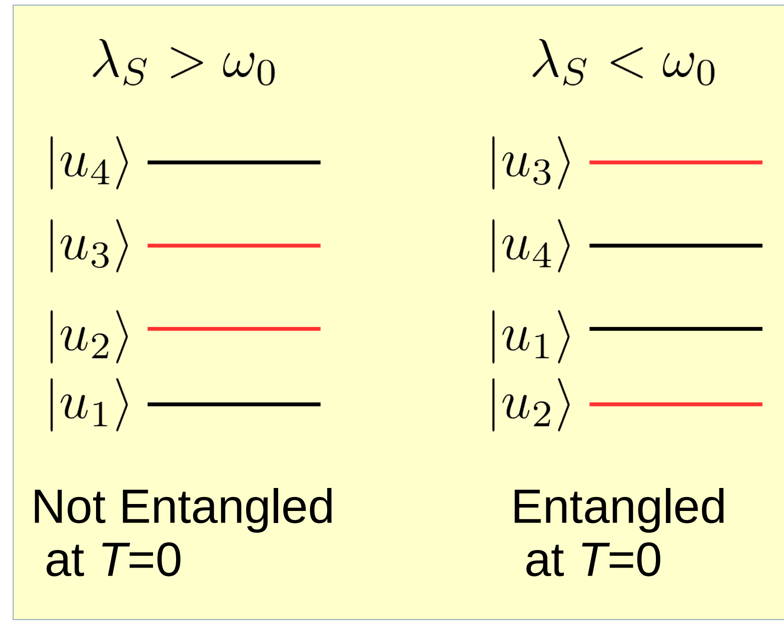
$$\hat{H}_S = \frac{\omega_0}{2}\hat{\sigma}^z_{S_1} + \frac{\omega_0}{2}\hat{\sigma}^z_{S_2} + \lambda_S\left(\hat{\sigma}^+_{S_1}\hat{\sigma}^-_{S_2} + \hat{\sigma}^-_{S_1}\hat{\sigma}^+_{S_2}\right)$$

$$E_1 = -\lambda_S, \quad |u_1\rangle = |--\rangle$$

$$E_2 = -\omega_0, \quad |u_2\rangle = \frac{1}{\sqrt{2}}\left(|+-\rangle - |-+\rangle\right)$$

$$E_3 = +\omega_0, \quad |u_3\rangle = \frac{1}{\sqrt{2}}\left(|+-\rangle + |-+\rangle\right)$$

$$E_4 = +\lambda_S, \quad |u_4\rangle = |++\rangle$$



Boson Baths

$$\hat{H}_{B_i} = \sum_k \omega_{B_i}(k)\,\hat{a}^\dagger_{B_i}(k)\hat{a}_{B_i}(k), \qquad i = 1, 2$$

System-Bath Coupling

$$\hat{V}_{S_iB_i} = \hat{X}_{S_i} \otimes \hat{Y}_{B_i}$$

$$\hat{X}_{S_i} = \sigma^+_{S_i} + \sigma^-_{S_i}$$

$$\hat{Y}_{B_i} = \sum_k \epsilon_{B_i}(k)\left[\hat{a}^\dagger_{B_i}(k) + \hat{a}_{B_i}\right]$$

Drude-Lorenzian model

$$g_{B_i}(\omega) = \sum_k |\epsilon_{B_i}(k)|\delta\left(\omega - \omega_{B_i}(k)\right)$$

$$= \frac{2\lambda_{B_i}\gamma_{B_i}\omega}{\omega^2 + \gamma^2_{B_i}}$$

General Solution to System Density

Unitary Evolution of the total system

$$\rho_{SB}(t) = \left\{ \overleftarrow{T} \prod_i e^{-i\int_{t_0}^{t} \hat{V}_{S_i B_i}(s)\mathrm{d}s} \right\} \rho_{SB}(t_0) \left\{ \overrightarrow{T} \prod_i e^{i\int_{t_0}^{t} \hat{V}_{S_i B_i}(s)\mathrm{d}s} \right\}$$

Initial state: $\rho_{SB}(t_0) = \rho_S(t_0) \otimes \rho_{B1}(t_0) \otimes \rho_{B_2}(t_0)$

Wick's theorem works: $\rho_{B_i}(t_0)$ is a quasi-free state. $\rho_{B_i}(t_0) = \frac{1}{Z_i} e^{-\beta_i \hat{H}_{B_i}}$

$$\rho_S(t) = \mathrm{tr}_{B_i}\left[\rho_{SB}(t)\right] = \overleftarrow{\mathcal{T}} \prod_i e^{-\int_{t_0}^{t}\int_{t_0}^{t_1} \mathrm{d}t_1 \mathrm{d}t_2 \mathcal{K}_i(t_1,t_2)} \rho_S(t_0)$$

$$\mathcal{K}_i(t_1, t_2) = \mathcal{S}_i^-(t_1)\ \mathrm{Im}\, C_i(t_1 - t_2)\, \mathcal{S}_i^-(t_2) + i\mathcal{S}_i^-(t_1)\ \mathrm{Re}\, C_i(t_1 - t_2), \mathcal{S}_i^+(t_2)$$

$$\mathcal{S}_i^{\pm}(t) = \left[\hat{X}_{S_i}(t),\ \cdot\ \right]_{\pm}$$

$$C_i(t) = \left\langle \hat{Y}_{B_i}(t)\hat{Y}_{B_i}(t_0)\right\rangle_0 \approx \lambda_{B_i}\left[c_i e^{-\gamma_{B_i} t} + 2\Delta_i \delta(t)\right]$$

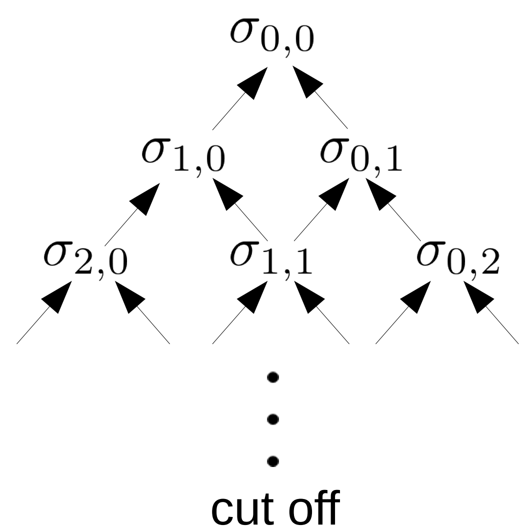
$$c_i = 2/\beta_i - \gamma_{B_i}(\Delta_i + \imath) \qquad \Delta_i =_{B_i} \beta_i/6$$

Hierarchical Equation of Motion (HEOM)

Auxiliary operators

$$\sigma_{n_1,n_2}(t) = \overleftarrow{\mathcal{T}} \prod_i \left\{ \left[-i \int_{t_0}^{t} \mathrm{d}s \, e^{-\gamma_{B_i}(t-s)} \mathcal{G}_i(s) \right]^{n_i} \times e^{-\lambda_{B_i} \int_{t_0}^{t} \int_{t_0}^{t_1} \mathrm{d}t_1 \mathrm{d}t_2 \mathcal{S}_i^-(t_1) e^{-\gamma_{B_i}(t_1-t_2)} \mathcal{G}_i(t_2)} \times e^{-\lambda_{B_i} \Delta_i \int_{t_0}^{t} \mathrm{d}t_1 \mathcal{S}^-(t_1) \mathcal{S}^-(t_1)} \right\} \rho_S(t_0)$$

$$\rho_S = \sigma_{0,0}$$



$$\mathcal{G}_i(t) = (2/\beta_i - \gamma_{B_i} \Delta_i) \, \mathcal{S}^-(t) - i \gamma_{B_i} \mathcal{S}^+(t).$$

Equation of Motion

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \sigma_{n_1,n_2}(t) &= -(\gamma_{B_1} n_1 + \gamma_{B_2} n_2) \, \sigma_{n_1,n_2}(t) \\ &- \left[\lambda_{B_1} \Delta_1 S_1^-(t) S_1^-(t) + \lambda_{B_2} \Delta_2 S_2^-(t) S_2^- t) \right] \sigma_{n_1,n_2}(t) \\ &- \imath \, \lambda_{B_1} \mathcal{S}_1^- \sigma_{n_1+1,n_2}(t) - \imath \, \lambda_{B_2} \mathcal{S}_2^- \sigma_{n_1,n_2+1}(t) \\ &- \imath \, n_1 \lambda_{B_1} \mathcal{G}_1(t) \sigma_{n_1-1,n_2}(t) - \imath \, n_2 \lambda_{B_2} \mathcal{G}_2(t) \sigma_{n_1,n_2-1}(t) \end{aligned}$$

HEOM is in principle exact.

- Correct description of coherence within the system
- Coherence with environment including entanglement.
- Strong coupling.

Heat Current

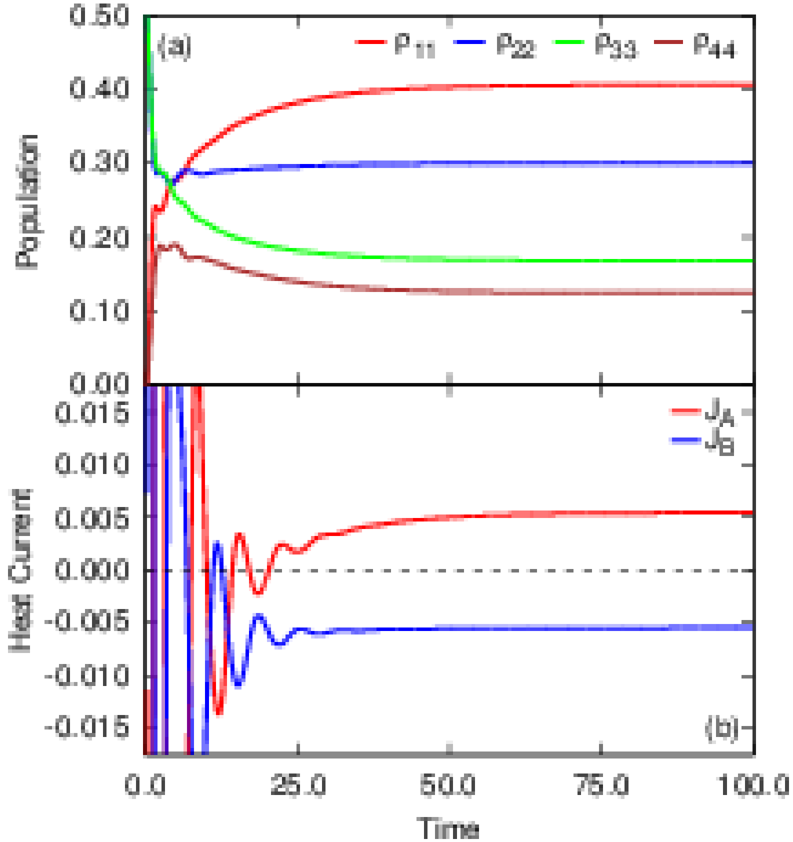
$$J_i = -\frac{\mathrm{d}}{\mathrm{d}t}\langle H_{B_i}\rangle = -\imath\,\mathrm{tr}_S\left\{[\hat{X}_{S_i}, \eta_i]\hat{H}_S\right\}$$

$$\eta_1 = \lambda_{B_1}\left\{\sigma_{1,0} - \imath\,\Delta_1 \mathcal{S}_1^- \sigma_{0,0}\right\}$$

$$\eta_2 = \lambda_{B_2}\left\{\sigma_{0,1} - \imath\,\Delta_2 \mathcal{S}_2^- \sigma_{0,0}\right\}$$

Numerical Calculation Procedure
(Exact enumeration in principle)

- Initial condition: $\sigma_{0,0}(t_0) = \rho_S(t_0), \quad \sigma_{i,j}(t_0) = 0$
- Hierarchic cut-off: $\sigma_{i,j}(t) = 0 \text{ for } i > i_{\max}, j > j_{\max}$
- Solve coupled ODEs (HEOM) numerically
- Non-Markovian solution: $\rho_S(t) = \sigma_{0,0}(t)$



$\omega_0 = 1, \quad \lambda_S = 0.5$

$\lambda_{B_1} = \lambda_{B_2} = 0.1$

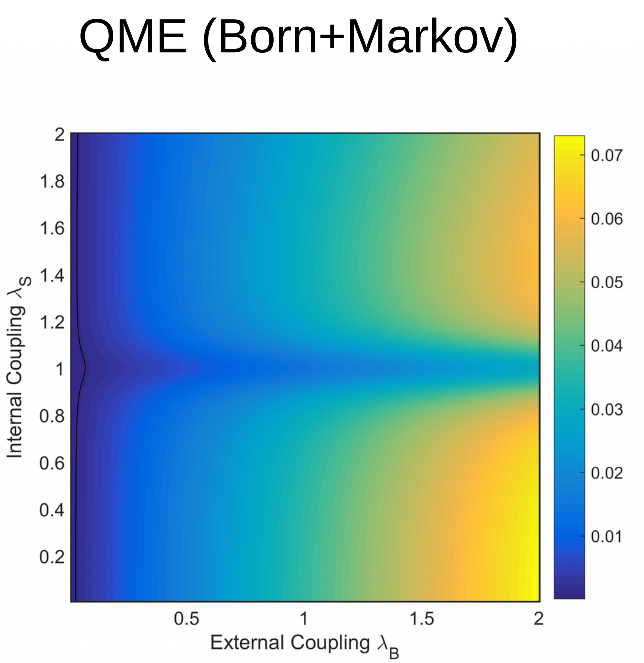
$\gamma_{B_1} = 0.2, \quad T_1 = 2$

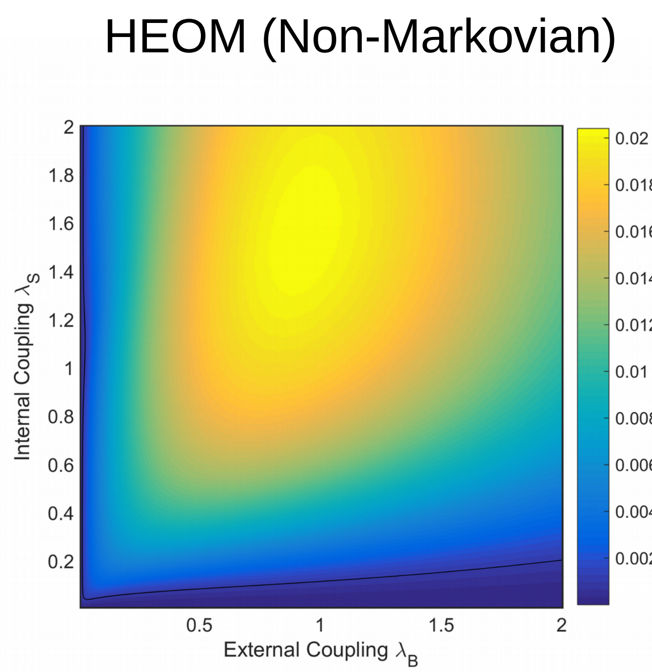
$\gamma_{B_2} = 0.1, \quad T_2 = 1$

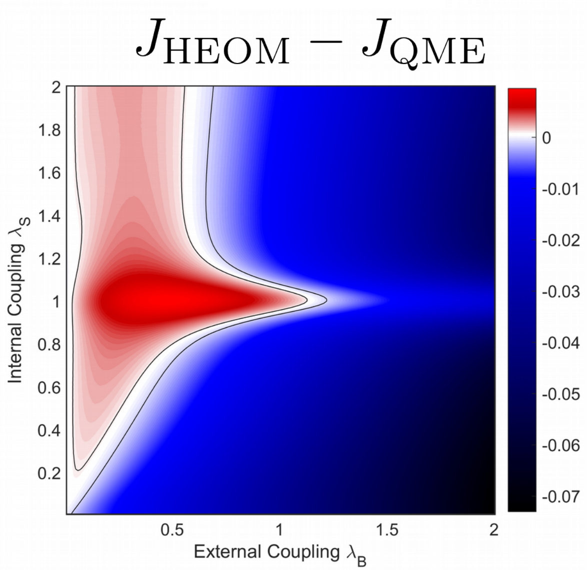
Hierarchy depth = 20

Comparison between QME and HEOM

Heat Current



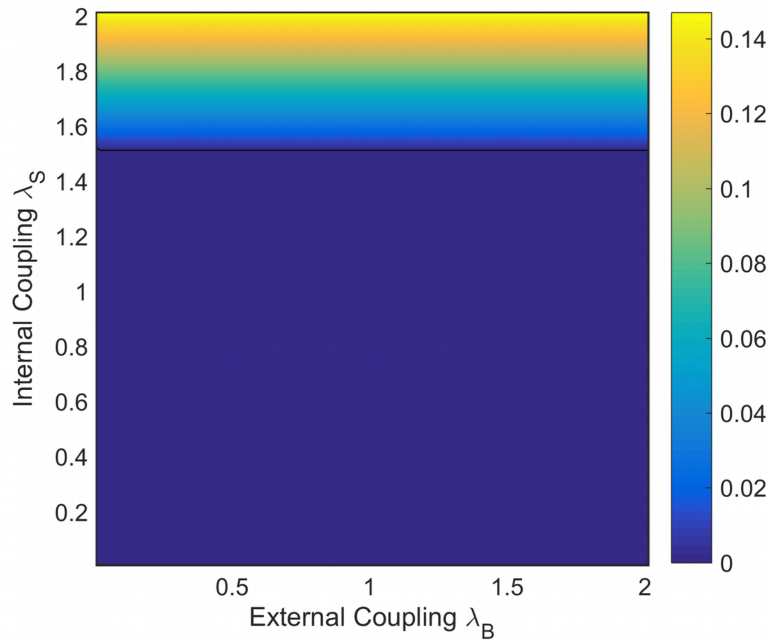




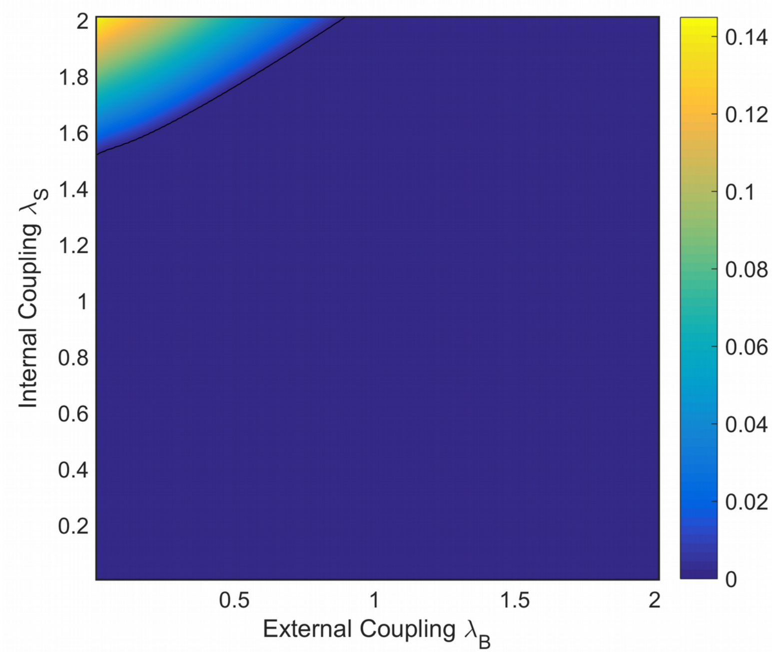
Comparison between QME and HEOM

Entanglement between Q-bits

QME (Born+Markov)



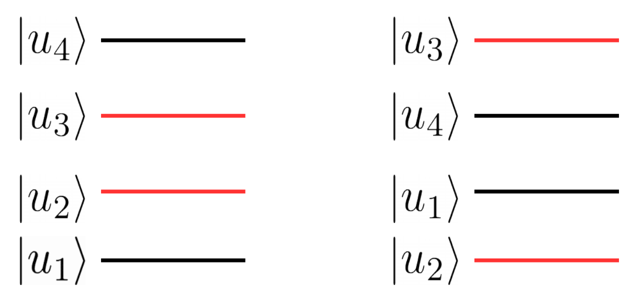
HEOM (Non-Markovian)

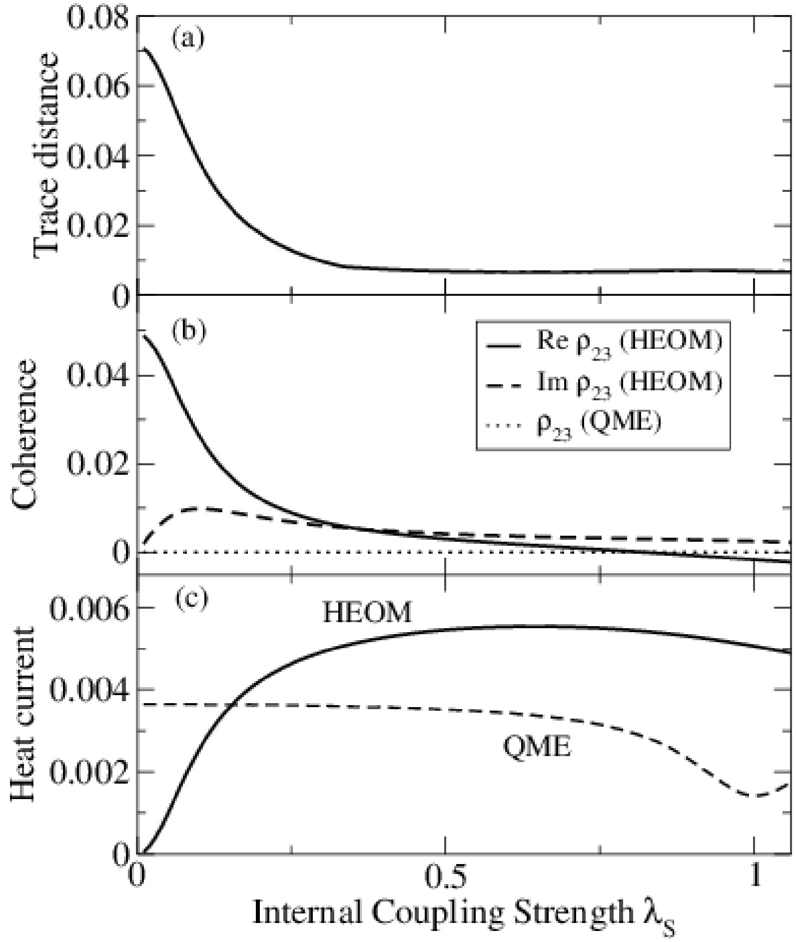


Concurrence $\quad C(\rho) = \max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4)$

λ_i = eigenvalue of $R = \sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}}$ in decreasing order

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)$$





Trace distance = $\|\rho - \sigma\| = \frac{1}{2}\,\mathrm{tr}\left[\sqrt{(\rho-\sigma)^\dagger(\rho-\sigma)}\right]$

Autonomous Quantum Heat Engine