Quantum thermodynamics of adiabatic processes

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Outline

- Quantum thermodynamics
- Adiabatic processes in classical thermodynamics and quantum thermodynamics
- Non-isolated adiabatic processes in quantum thermodynamics
- Set-up for non-isolated adiabatic processes
- Comparison with the conventional adiabatic processes
- Future outlook

Quantum Thermodynamics (QT)

- Quantum thermodynamics is the study of Thermodynamics for Quantum Systems.

In the quantum regime → the concepts of heat, work, and temperature
→ laws of thermodynamics are derived

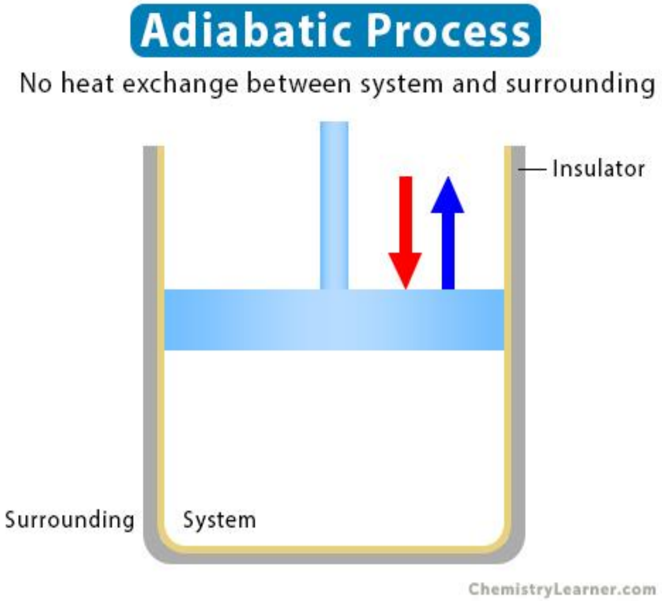
- The central goal is to extend standard thermodynamics to include small system sizes and quantum effects.

small system sizes → Fluctuations of heat and work
quantum effects → quantum superposition,
quantum correlation (quantum information)

- Quantum thermodynamic processes → Quantum Isothermal, **Quantum Adiabatic**, Quantum Isochoric

Adiabatic Processes in Classical Thermodynamics

In adiabatic processes, **the system does not exchange energy with the environment in the form of heat.**



In adiabatic processes, the **entropy of the system can change**.

Adiabatic processes here are different from mechanical adiabaticity.

Adiabatic Processes in Quantum Thermodynamics

Adiabatic processes commonly mean processes in **isolated systems** given by unitary evolution by a time-dependent Hamiltonian.

$\hat{\rho}_S(\mathrm{t}) = \hat{U}(t)\hat{\rho}_S(0)\hat{U}^{\dagger}(t)$ where $\hat{U}(t) = \vec{\mathcal{T}} e^{-i\int_o^t dt'\hat{H}_S(t')}$

The system's von Neumann **entropy remains conserved** in the isolated processes.

Common wisdom: **"Adiabatic processes" = "Isolated Processes"**

Non-isolated Adiabatic Processes in Quantum Thermodynamics

Adiabatic processes are not necessarily the processes in the isolated systems:

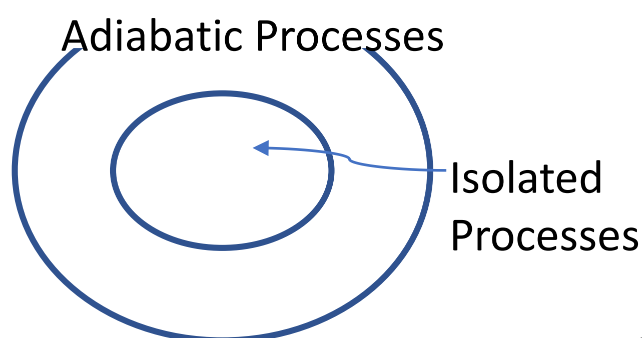
Adiabatic processes $\neq$ Isolated Processes

For quantum systems, **Isolation is a sufficient condition** for the adiabatic processes, but **it is not a necessary condition**.

There exist adiabatic processes which are not isolated ones for the quantum case.

Examples: **"Decoherence"** or **"Dephasing"**

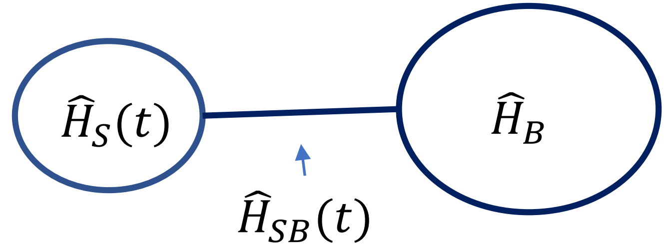
Non-isolated adiabatic processes



Set-Up for Non-isolated Adiabatic Processes

Hamiltonian:

$$\hat{H}(t) = \hat{H}_S(t) + \hat{H}_B + \hat{H}_{SB}(t)$$



$$\hat{H}_{SB}(t) = \sum_m g_m(t)\, \hat{\Pi}_m^S(t) \otimes \hat{V}_m$$

Label of sys. basis (m = e, g)

Bath opt.

Condition: $[\hat{H}_B, \hat{V}_m] = 0$

$$\rightarrow [\hat{H}_{SB}(t), \hat{H}(t)] = 0$$

Heat in Non-isolated Adiabatic Processes

Heat is defined by the energy change in the bath.

Initial state: $\hat{\rho}(0) = \hat{\rho}_S(0) \otimes \hat{\rho}_B(0)$

Non-diagonal in $\widehat{H}_S(0)$ basis

Diagonal in $\widehat{H}_B(0)$ basis

Using $[\widehat{H}_B, \widehat{H}_{SB}(t)] = 0$ $\Longrightarrow$ $P(Q) = \delta(Q)$

Heat Q = 0 deterministically without fluctuation.

Time Evolution of the System in Non-isolated Adiabatic Processes

$$\hat{\rho}(\mathrm{t}) = U(t)\hat{\rho}(0)\hat{U}^{\dagger}(t) \quad \text{where} \quad U(t) = \vec{\mathcal{T}} e^{-i\int_o^t dt' H(t')}$$

System's state: $\hat{\rho}_S(\mathrm{t}) = Tr_B[\hat{\rho}(\mathrm{t})]$

Using $[\hat{H}_B, \hat{H}_{SB}(t)] = 0$

$$\hat{\rho}_S(t) = \sum_i \hat{M}_i(t)\,\hat{\rho}_S(0)\hat{M}_i{}^{\dagger}(t)$$

The map $\mathcal{E}$: $\mathcal{E}\big(\hat{\rho}_S(0)\big) = \sum_i \hat{M}_i(t)\,\hat{\rho}_S(0)\hat{M}_i^{\dagger}(t)$ makes $\hat{\rho}_S(0) \to \hat{\rho}_S(\mathrm{t})$.

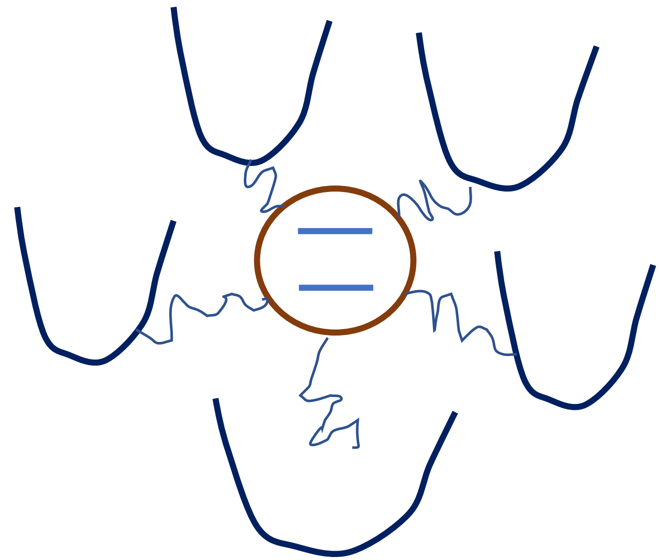
$\mathcal{E}$ trace preserving map: $Tr_S\big(\hat{\rho}_S(\mathrm{t})\big) = Tr_S\big(\hat{\rho}_S(0)\big)$

$\mathcal{E}$ unital map: $\mathcal{E}\big(\hat{\mathbb{I}}_S\big) = \sum_i \hat{M}_i(t)\,\hat{\mathbb{I}}_S \hat{M}_i^{\dagger}(t) = \hat{\mathbb{I}}_S$

$\mathcal{E}$ is a trace − preserving and unital Kraus map.

Demonstration with the Specific Model

A two level system in a HO bath $\hat{H}_S(t) = \frac{\omega_S(t)}{2}\hat{\sigma}_z$ $\hat{H}_B = \sum_\mu \omega_\mu \hat{a}_\mu{}^\dagger \hat{a}_\mu$



Under the condition: $[\,\hat{H}_{SB}(t), \hat{H}(t)\,] = 0$

From the Kraus map:

$$\hat{\rho}_S(t) = \sum_{j=0}^{\infty} p_{B,j}^{(N)}(0)\ \{\, p_{S,ee}(0)|e\rangle\langle e| + p_{S,gg}(0)|g\rangle\langle g| + e^{i[\bar{\omega}_S(t) + (\bar{g}_e(t) - \bar{g}_g(t))j\,]t}\, p_{S,ge}(0)|g\rangle\langle e| + e^{-i[\bar{\omega}_S(t) + (\bar{g}_e(t) - \bar{g}_g(t))j\,]t}\, p_{S,eg}(0)|e\rangle\langle g| \,\}$$

$$\bar{\omega}_S(t) = \frac{1}{t}\int_0^t dt'\omega_S(t') \qquad \bar{g}_m(t) = \frac{1}{t}\int_0^t dt' g_m(t') \quad \text{(m = e, g)}$$

Unitary Evolution Versus Non-isolated Processes

$$\hat{\rho}_S(\mathrm{t}) = \hat{U}(t)\hat{\rho}_S(\mathrm{t})\hat{U}^\dagger(t) \qquad \text{where} \qquad \hat{U}(t) = \vec{\mathcal{T}} e^{-i\int_o^t dt' \hat{H}_S(t\prime)}$$

$$\hat{\rho}_S(t) = p_{S,ee}(0)|e\rangle\langle e| + p_{S,gg}(0)|g\rangle\langle \mathrm{g}| + e^{-i\,\bar{\omega}_S(t)\,t}\, p_{S,eg}(0)|e\rangle\langle \mathrm{g}| + e^{i\,\bar{\omega}_S(t)\,t}\, p_{S,ge}(0)|g\rangle\langle e|$$

If $\hat{\rho}_S(0)$ is diagonal in the $\hat{H}_S$ basis: $p_{S,eg}(0) = p_{S,ge}(0) = 0$

$$\hat{\rho}_S(t) = p_{S,ee}(0)|e\rangle\langle e| + p_{S,gg}(0)|g\rangle\langle \mathrm{g}|$$

The state $\hat{\rho}_S(t)$ is the same for the non-isolated process and the unitary evolution case.

The time evolved state $\hat{\rho}_S(t)$ will be different for two cases if the initial $\hat{\rho}_S(0)$ is non-diagonal in the $\hat{H}_S$ basis.

Entropy Change of the System

Von Neumann entropy : $S(\hat{\rho}_S(t)) = -Tr(\hat{\rho}_S(t)\ln(\hat{\rho}_S(t))) = -(\lambda_+ ln\lambda_+ + \lambda_- ln\lambda_-)$

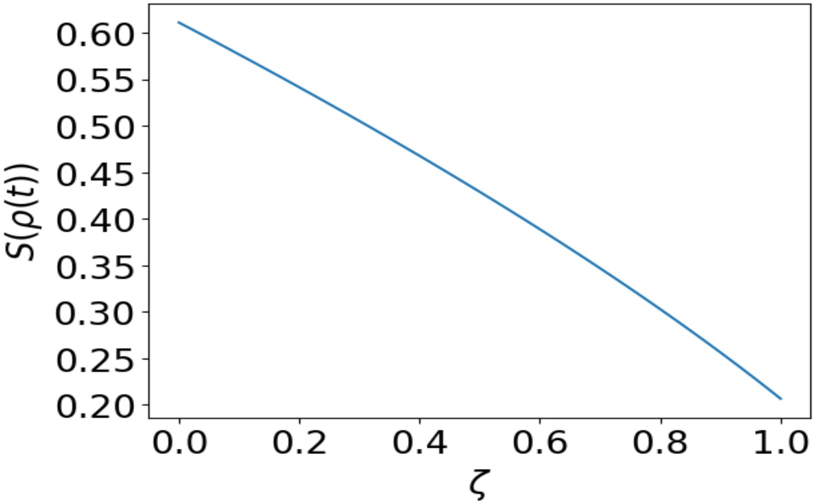
Eigen values: $\lambda_\pm = \frac{1}{2}\left(1 \pm \sqrt{(1-2p_e)^2 + 4|a|^2}\right)$

$$|a|^2 = \left|p_{S,eg}(0)\right|^2 \zeta$$

Unitary evolution case: $\zeta = 1 \rightarrow |a|^2 = \left|p_{S,eg}(0)\right|^2$

The factor ζ characterizes the difference between non-isolated adiabatic processes and unitary evolution case.

In general: $0 \leq \zeta \leq 1$



Future Outlook

- **Average work and fluctuation of work under a non-isolated setup**

  ➡ The effect of the coherence will be suppressed and the system will be close to the quasi-static state under the non-isolated setup.

Thank you

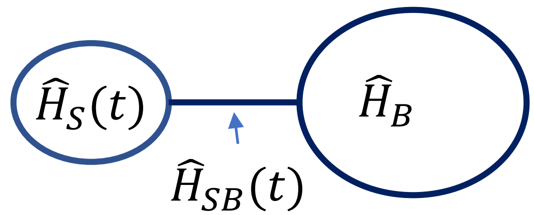
Questions?

Set-Up for Non-isolated Adiabatic Processes

Hamiltonian:

$$\hat{H}(t) = \hat{H}_S(t) + \hat{H}_B + \hat{H}_{SB}(t)$$

$$\hat{H}_S(t) = \sum_n \varepsilon_n(t)\hat{\Pi}_n^S(\mathrm{t})$$



$$\hat{H}_B = \sum_i E_i \hat{\Pi}_i^B$$

$$\hat{H}_{SB}(t) = \sum_m g_m(t)\, \hat{\Pi}_m^S(t) \otimes \hat{V}_m$$

Label of sys. basis (→ m)

Bath opt. (→ $\hat{V}_m$)

Condition: $[\hat{H}_B, \hat{V}_m] = 0$ for ∀ m , (m = e, g)

$$[\hat{H}_{SB}(t), \hat{H}(t)] = 0$$

Initial state: $\hat{\rho}(0) = \hat{\rho}_S(0) \otimes \hat{\rho}_B(0)$

Non-diagonal in $\hat{H}_S(0)$ basis

Diagonal in $\hat{H}_B(0)$ basis

Heat in Non-isolated Adiabatic Processes

Heat: It is defined by the energy change in the bath measured by 2-point energy measurement.

Joint probability of the bath's state i → j

$$p_B(ij) = p_{B,i}p_{B,ji} = Tr[\hat{\Pi}_j^B \vec{\mathcal{T}} e^{-i\int_o^t dt' H(t')} \hat{\Pi}_i^B \hat{\rho}(0) \hat{\Pi}_i^B \overleftarrow{\mathcal{T}} e^{i\int_o^t dt' H(t')} \hat{\Pi}_j^B]$$

Heat distribution function: $P(Q) = \sum_{ij} \delta\left(Q - (E_j - E_i)\right) p_{ij}(B)$

Characteristic function: $\Theta(u) = \int_{-\infty}^{\infty} dQ\, e^{iuQ} P(Q)$

Using $[\hat{H}_B, \hat{V}_m] = 0$ ⇨ $\Theta(u) = 1$

$P(Q) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dQ\, e^{-iuQ}\Theta(u) =$
$\delta(Q)$

Heat Q = 0 deterministically without fluctuation.

Time evolution of the system in Non-isolated Adiabatic Processes

$$\hat{\rho}_S(\mathrm{t}) = Tr_B[\vec{\mathcal{T}} e^{-i\int_o^t dt' H(t')} \hat{\rho}(0)\, \overleftarrow{\mathcal{T}} e^{i\int_o^t dt' H(t')}]$$

Using $[\hat{H}_B, \hat{V}_m] = 0$

$$\hat{\rho}(\mathrm{t}) = \sum_i \hat{M}_i(t)\, \hat{\rho}_S(0) \hat{M}_i{}^\dagger(t)$$

Kraus op. $\hat{M}_i(t) = \sqrt{p_{B,i}(0)}\;\; \vec{\mathcal{T}} e^{-i\int_o^t dt' H_S(t') + \sum_m g_m(t)\, \nu_{m,i}\, \hat{\Pi}_m^S}$

$$\sum_i \hat{M}_i(t)\, \hat{M}_i^\dagger(t) = \hat{\mathbb{I}}_S$$

The map $\mathcal{E}$: $\mathcal{E}\big(\hat{\rho}_S(0)\big) = \sum_i \hat{M}_i(t)\, \hat{\rho}_S(0) \hat{M}_i^\dagger(t)$ makes $\hat{\rho}_S(0) \to \hat{\rho}_S(\mathrm{t})$.

$\mathcal{E}$ trace preserving map: $Tr_S\big(\hat{\rho}_S(\mathrm{t})\big) = Tr_S\big(\hat{\rho}_S(0)\big)$

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$\mathcal{E}$ is a trace − preserving and unital Kraus map.

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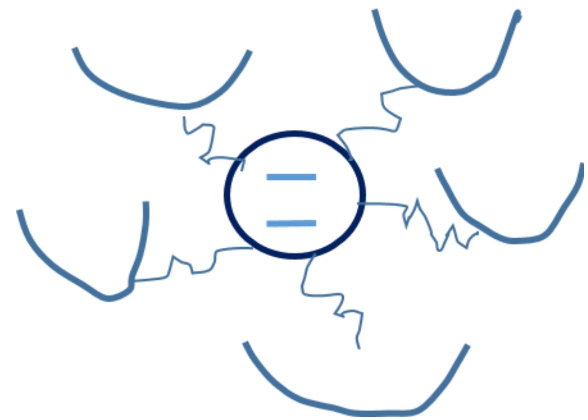
A two level system in a HO bath $\quad \hat{H}_S(t) = \frac{\omega_S(t)}{2}\hat{\sigma}_z \quad \hat{H}_B = \sum_\mu \omega_\mu \hat{a}_\mu{}^\dagger \hat{a}_\mu$

$$\hat{H}_{SB}(t) = \left(g_e(t)|e\rangle\langle e| + g_g(t)|g\rangle\langle g|\right)\sum_\mu f_\mu \hat{a}_\mu{}^\dagger \hat{a}_\mu$$



Under the condition: $\quad [\,\hat{H}_{SB}(t), \hat{H}(t)\,] = 0$

From the Karaus map:

$$\hat{\rho}_S(t) = \sum_{j=0}^{\infty} p_{B,j}^{(N)}(0)\ \{\, p_{S,ee}(0)\ |e\rangle_{SS}\langle e| + p_{S,gg}(0)\ |g\rangle_{SS}\langle g| + e^{i[\bar{\omega}_S(t) + (\bar{g}_e(t)-\bar{g}_g(t))j\,]t}\ p_{S,ge}(0)\ |g\rangle_{SS}\langle e| + e^{-i[\bar{\omega}_S(t) + (\bar{g}_e(t)-\bar{g}_g(t))j\,]t}\ p_{S,eg}(0)\ |e\rangle_{SS}\langle g|\,\}$$

$$\bar{\omega}_S(t) = \frac{1}{t}\int_0^t dt'\omega_S(t') \qquad \bar{g}_m(t) = \frac{1}{t}\int_0^t dt' g_m(t') \quad \text{(m = e, g)}$$