

Trajectory-based GKLS equation and its energetics

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[1] Quantum 4, 336 (2020)

[2] arXiv:1912.01939

1- starting from maps: CPTP/q channels

$$\varrho(\tau_2) = \mathcal{E}_s(\tau_2, \tau_1)[\varrho(\tau_1)]$$

- —no initial correlation
- —time homogeneous **dynamical semigroup** property

(divisibility of the dynamical map)

$$\mathcal{E}_S(\tau_1 + \tau_2) = \mathcal{E}_S(\tau_2)\mathcal{E}_S(\tau_1)$$

$$\mathcal{L}_{S}\varrho_{S}(\tau) = -i[\widetilde{H}_{S}, \varrho_{S}(\tau)] + \sum_{m} \gamma_{m} \left(2L_{m}\varrho_{S}L_{m}^{\dagger} - \{L_{m}^{\dagger}L_{m}, \varrho_{S}\}\right)$$



1'- more general: starting from maps (without semigroup property with memory effects)

Gorini-Kossakowski-Sudarshan theorem

no initial correlation

Any linear map with Hermiticity and trace preserving properties can be associated to a time-local generator as

$$\mathcal{L}_{S}\varrho_{S}(\tau) = -i[\widetilde{H}_{S}, \varrho_{S}(\tau)] + \sum_{m} \gamma_{m} \left(2L_{m}\varrho_{S}L_{m}^{\dagger} - \{L_{m}^{\dagger}L_{m}, \varrho_{S}\} \right)$$

[M. Merkli's talk]

can be negative

[G. A. Paz-Silva et al., Phys. Rev. A 100, 042120 (2019)]

2- starting from Hamiltonian (microscopic derivation)

- —Born approximation $\varrho_{SB}(\tau) = \varrho_{S}(\tau) \otimes \varrho_{B}(0)$ $(\tau_{S} \gg \tau_{B})$
- -Markov approximation (killing the dependence of time evolution of the state on the state at earlier times)
- —Rotating wave approximation (RWA) (fast oscillating terms are neglected)



Markovian master equation

$$\mathcal{L}_{S}\varrho_{S}(\tau) = -i[\widetilde{H}_{S}, \varrho_{S}(\tau)] + \sum_{m} \gamma_{m} \left(2L_{m}\varrho_{S}L_{m}^{\dagger} - \{L_{m}^{\dagger}L_{m}, \varrho_{S}\} \right)$$

2'- more general: starting from Hamiltonian (microscopic derivation)

correlation-picture approach

universal GKSL dynamical equation for general open quantum system

$$\dot{\varrho}_{\mathsf{S}} = \mathcal{L}^{\chi}[\varrho_{\mathsf{S}}] = -i[H_{\mathsf{S}} + \mathbb{h}_{\mathsf{L}}^{\chi}, \varrho_{\mathsf{S}}] + \sum \gamma_{m}^{\chi} \left(2L_{m}^{\chi}\varrho_{\mathsf{S}}L_{m}^{\chi\dagger} - \{L_{m}^{\chi\dagger}L_{m}^{\chi}, \varrho_{\mathsf{S}}\}\right)$$

[Phys. Rev. X **10**, 041024 (2020)] j joint work with A. T. Rezakhani, A. Babu, K. Mølmer, M. Möttönen, T. Ala-Nissila

key element: $\varrho_{SB} = \varrho_{S} \otimes \varrho_{B} + \chi$

general:

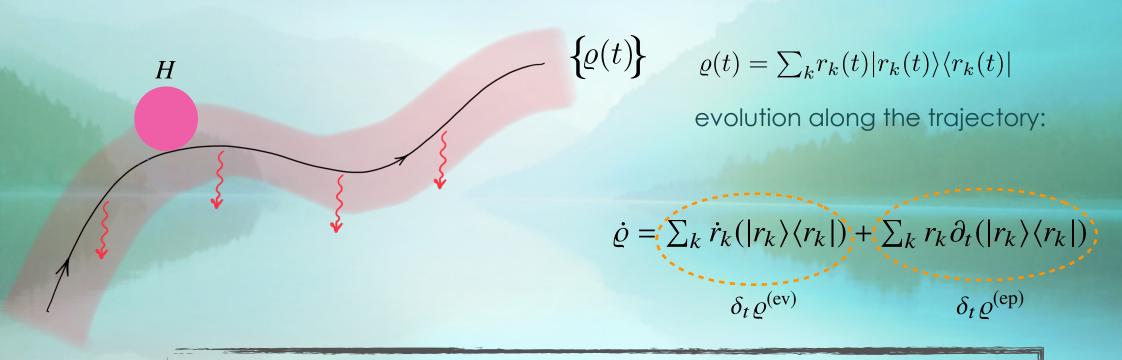
no weak-coupling

no Markovian

no uncorrelated preparation assumptions

[M. J. W. Hall et al., Phys. Rev. A 89, 042120 (2014)][D. Chruściński et al., Phys. Rev. Lett. 104, 070406 (2010)]

3- trajectory-based approach

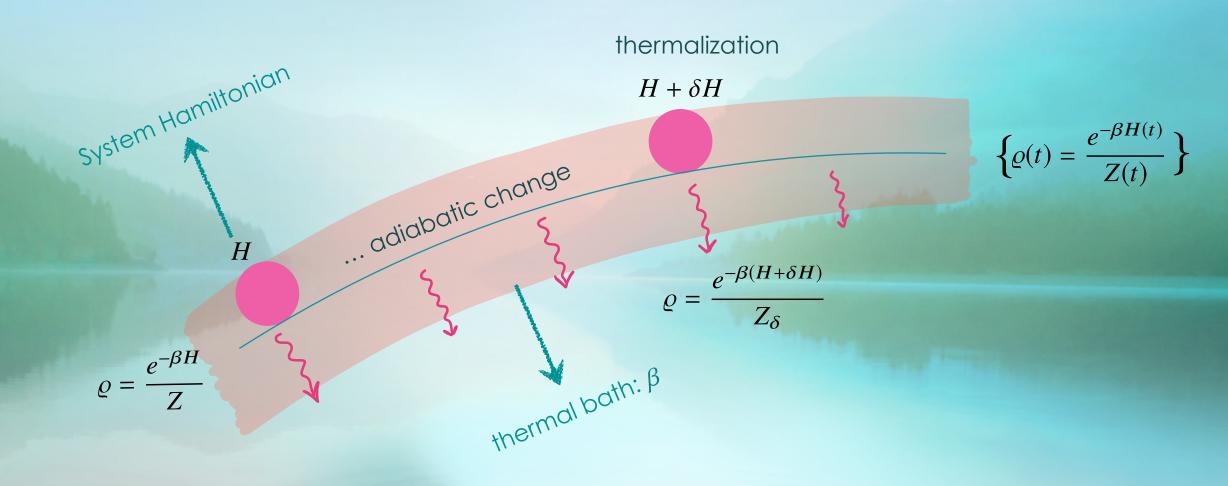


is it possible to assign a GKLS equation to any given trajectory?

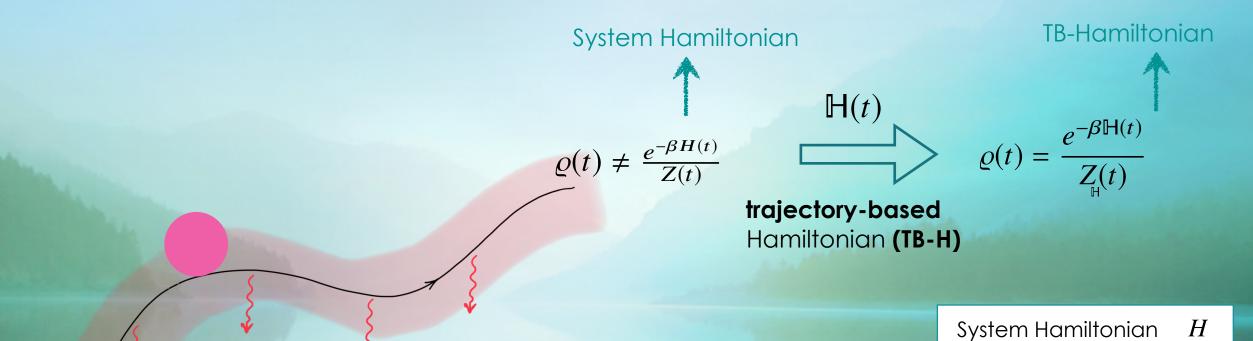
disclaimer:

the goal **IS NOT** to provide a microscopic/physical prescription to realize a particular trajectory

special case: thermal trajectory for a system in contact with a thermal bath



general case: the given trajectory is non-thermal



TB-Hamiltonian

 \mathbb{H}

key observation: arbitrary trajectory = "thermal" trajectory

goal: setting up a scenario such that the given trajectory is $\left\{\varrho(t) = \frac{e^{-\beta \mathbb{H}(t)}}{Z(t)}\right\}$

$$\left\{ \varrho(t) = \frac{e^{-\beta \mathbb{H}(t)}}{Z(t)} \right\}$$

achieving this goal in two steps:

$$\delta_t \varrho^{\text{(ev)}} \qquad \delta_t \varrho$$

$$\dot{\varrho} = \sum_k \dot{r}_k (|r_k\rangle\langle r_k|) + \sum_k r_k \partial_t (|r_k\rangle\langle r_k|)$$

1- description of the change in the eigenvectors

- now prepare a system with TB-Hamiltonian H with no environment around
- assume adiabatic change of TB-H

dynamics:

S:
$$\widetilde{\varrho}(t+\delta t) \neq \frac{e^{-\beta \mathbb{H}(t+\delta t)}}{Z(t+\delta t)}$$

$$\varrho(t) = \frac{e^{-\beta \mathbb{H}(t)}}{Z(t)}$$

$$\varrho(t) = \frac{e^{-\beta \mathbb{H}(t)}}{Z(t)}$$

dynamics:

$$\mathbb{H}(t) = \sum_{k} \epsilon_k(t) |r_k(t)\rangle \langle r_k(t)|$$

$$|r_k(t)
angle \ \ \, pprox |r_k(t+\delta t)
angle$$

$$\varrho(t) = \frac{e^{-\beta \mathbb{H}(t)}}{Z(t)}$$

$$\varrho(t) = \sum_{k} r_k(t) |r_k(t)\rangle \langle r_k(t)|$$

$$\epsilon_i = -\beta^{-1} \log(r_i Z)$$

 $\delta_t \varrho^{(\mathrm{ev})}$

$$\widetilde{\varrho}(t+\delta t) = \sum_{k=1}^{g} |r_k(t)| |r_k(t+\delta t) \rangle \langle r_k(t+\delta t)|$$

$$H$$

$$H_{\text{CD}}$$

$$\partial_t \left(|r_k(t)\rangle \langle r_k(t)| \right) = -i \left[\mathbb{H}_{\mathrm{CD}}(t), |r_k(t)\rangle \langle r_k(t)| \right]$$

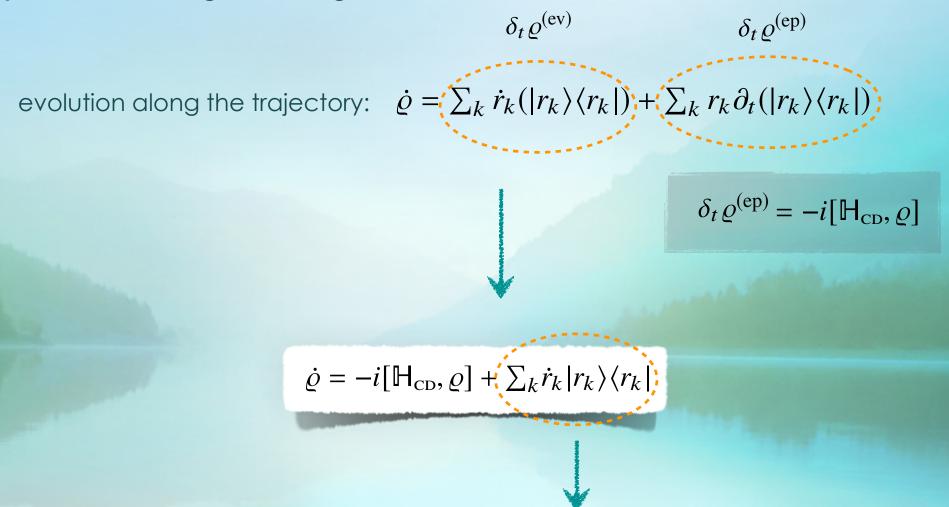
$$\mathbb{H}_{\mathrm{CD}} = \mathbb{H} + \mathbb{h} \qquad \mathbb{h} = i \sum_k \left(|\dot{r}_k\rangle \langle r_k| - \langle r_k|\dot{r}_k\rangle |r_k\rangle \langle r_k| \right)$$

$$\dot{\varrho} = \sum_{k} \dot{r}_{k} (|r_{k}\rangle\langle r_{k}|) + \sum_{k} r_{k} \partial_{t} (|r_{k}\rangle\langle r_{k}|)$$

 $\delta_t \varrho^{(\mathrm{ep})}$

$$\sum_{k} r_{k} \partial_{t}(|r_{k}\rangle\langle r_{k}|) = -i[\mathbb{H}_{CD}, \varrho] \equiv -i[\mathbb{h}, \varrho]$$

2- description of the change in the eigenvalues



description of this term in the GKLS form?

2- description change of the eigenvalues

envalues
$$\delta_t arrho^{
m (ev)}$$
 $\dot{arrho} = -i [\mathbb{H}_{ ext{CD}}, arrho] + \sum_k \dot{r}_k |r_k
angle \langle r_k|$

$$\varrho(t) = \sum_k r_k(t) |r_k(t)\rangle \langle r_k(t)|$$

$$\mathbb{H}(t) = \sum_k \epsilon_k(t) |r_k(t)\rangle \langle r_k(t)|$$

changing the eigenvalues = changing the probabilities of staying in a level

jump operators:

$$L_{kj} = |r_k\rangle\langle r_j|$$



rates:
$$\gamma_{kj} = \dot{r}_k/(g\,r_j)$$

$$\delta_t \varrho^{(\text{ev})} = \mathcal{D}[\varrho] = \sum_{ij} \gamma_{ij} \left(L_{ij} \varrho L_{ij}^{\dagger} - \frac{1}{2} \{ L_{ij}^{\dagger} L_{ij}, \varrho \} \right)$$

$$\dot{\varrho} = -i[\mathbb{H}_{CD}, \varrho] + \mathcal{D}[\varrho]$$



- general: no weak-coupling/no Markovian/no uncorrelated preparation assumptions
- **geometric** and trajectory-dependent
- no need for thermal environment
- no need to be full-rank

microscopically derived GKLS

TB-GKLS

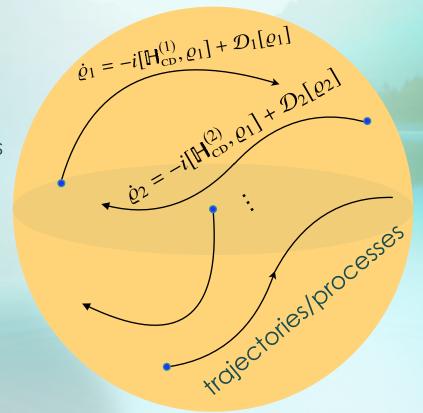
$$\dot{\varrho} = -i[H, \varrho] + \mathcal{L}[\varrho]$$

$$\dot{\varrho} = -i[\mathbb{H}_{CD}, \varrho] + \mathcal{D}[\varrho]$$

Hilbert space of the system

master equation for all trajectories

$$\dot{\varrho} = -i[H, \varrho] + \mathcal{L}[\varrho]$$



so far so good but

so what?

 natural application: dynamical and thermodynamic process engineering (not the subject of this talk)

energetics of TB-GKLS



unambiguous description of heat and work (thermodynamics)

energetics of microscopically derived GKLS

$$\dot{\varrho} = -i[H, \varrho] + \mathcal{L}[\varrho]$$



system Hamiltonian/effective Hamiltonian



Internal energy: $U = \text{Tr}[\varrho H]$

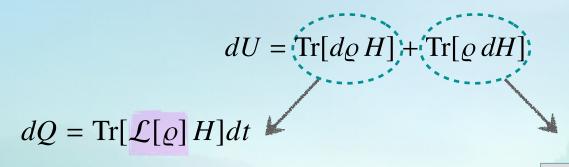
energy change: $dU = \text{Tr}[d\varrho H] + \text{Tr}[\varrho dH]$

no contribution to energy change by the coherent part $\text{Tr}[-i[H,\varrho]H]=0$

$$Tr[d\varrho H] = Tr[\mathcal{L}[\varrho]H]$$

heat and work in quantum regime: conventional definitions

[a la Alicki et al.]



dW (external) work

heat?

				\
pros	cons		work	
1— first law				F
dQ = dU - dW	dW whole work?	Н		change in energy levels (physical structure)

2— second law: entropy change

does the whole of $\mathcal{L}[\varrho]$ contributes to entropy change?

$$dS = -\text{Tr}[d\varrho \log \varrho]$$

$$dS = -\text{Tr}[d\varrho \log \varrho] \qquad \stackrel{\dot{\varrho} = -i[H, \varrho] + \mathcal{L}[\varrho]}{\partial S} \qquad \partial S = -\text{Tr}[\mathcal{L}[\varrho] \log \varrho] dt$$

what do we learn from the TB-GKLS?

energy change: $dU = \text{Tr}[d\varrho H] + \text{Tr}[\varrho dH]$

entropy change: $dS = -\text{Tr}[d\varrho \log \varrho]$

	TB-GKLS $\dot{\varrho} = -i[\mathbb{h}, \varrho] + \mathcal{D}[\varrho]$	microscopic $\dot{\varrho} = -i[H,\varrho] + \mathcal{L}[\varrho]$
$Tr[d\varrho H]$	$-i\operatorname{Tr}[[\mathbb{h},\varrho]H]dt + \operatorname{Tr}[\mathcal{D}[\varrho]H]dt$	$\mathrm{Tr}[\mathcal{L}[\varrho]H]dt$
dS	$-\mathrm{Tr}[\mathcal{D}[\varrho]\log\varrho]dt$	$-\mathrm{Tr}[\mathcal{L}[\varrho]\log\varrho]dt$

There is part of the energy exchange, in the dissipative part of the microscopic master equation, along the trajectory, which does not contribute in entropy change

dQ may have "non-heat" contributions

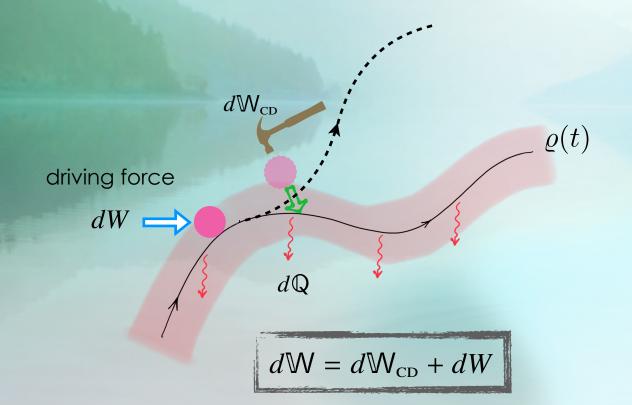
a closer look:

$$\dot{\varrho} = -i[\mathbb{h}, \varrho] + \mathcal{D}[\varrho]$$

$$d\varrho = \delta\varrho^{(\text{ep})} + \delta\varrho^{(\text{ev})}$$

$$\sum_{k} r_k d(|r_k\rangle\langle r_k|)$$

$$\sum_k dr_k(|r_k\rangle\langle r_k|)$$
 nonunitary, entropy change



$$dS = -\sum_{k} dr_{k} \ln r_{k} \equiv -\text{Tr}[\delta \varrho^{\text{(ev)}} \ln \varrho]$$

$$dU = \text{Tr}[\varrho \, dH] + \text{Tr}[d\varrho \, H]$$

$$\equiv \text{Tr}[\varrho \, dH] + \text{Tr}[\delta \varrho^{(\text{ep})}H] + \text{Tr}[\delta \varrho^{(\text{ev})}H]$$

$$\text{work} \qquad \text{work} \qquad \text{heat}$$

$$\text{trajectory-induced}$$

$$dW \qquad d\mathbb{W}_{\text{CD}} \qquad d\mathbb{Q}$$

 $\varrho(t) = \sum_{k} r_k(t) |r_k(t)\rangle \langle r_k(t)|$

 $\mathbb{H}(t) = \sum_{k} \epsilon_k(t) |r_k(t)\rangle \langle r_k(t)|$

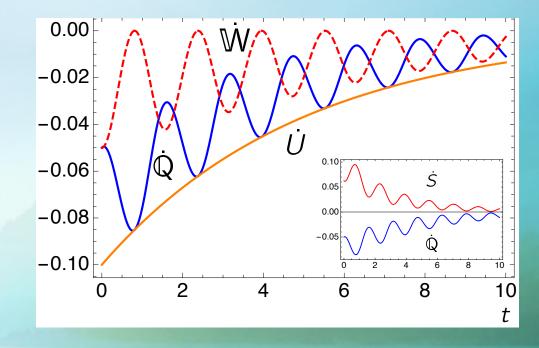
example: transversal noise

time-independent Hamiltonian

$$\dot{\varrho}(t) = -i[\omega_0 \sigma_z, \varrho(t)] + \gamma (\sigma_x \varrho(t) \sigma_x - \varrho(t))$$

$$\varrho(0) = (1/2)(1 + (\sigma_x + \sigma_z)/2)$$

$$\varrho(t) = \sum_{s=0,1} \frac{1 + (-1)^s e^{-2t\gamma} + \left(1 + (-1)^{s+1} e^{-2t\gamma}\right) e^{2\beta\omega_0}}{2(1 + e^{2\beta\omega_0})} |s\rangle\langle s|$$



is the heat exchange always accompanied by an entropy exchange?

example: dephasing

$$\dot{\varrho} = -i[\omega_0 \sigma_z, \varrho] + \gamma (\sigma_z \varrho \sigma_z - \varrho)$$

 $H=\omega_0\sigma_z$

energy is preserved: dU = 0

according to conventional definitions:

time-independent Hamiltonian no work
$$dW=0$$
 no energy, no work no heat $dQ=0$

for **any** initial state

$$1 - |\psi(0)\rangle = (|0\rangle + \sqrt{2}|1\rangle)/\sqrt{3}$$

$$\omega_0 = 1$$

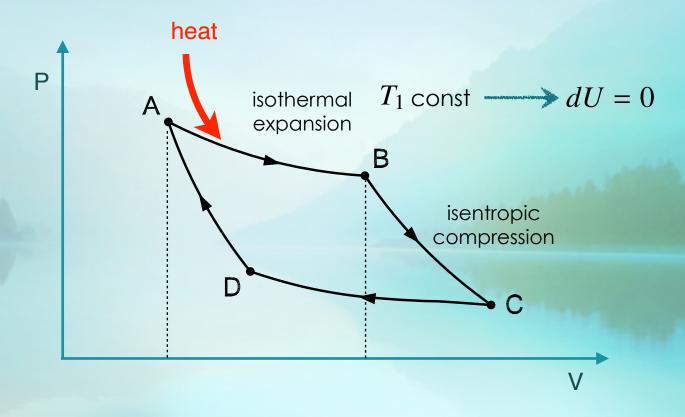
$$\gamma = 0.1$$

$$\dot{\mathbf{Q}} = -\dot{\mathbf{W}}_{CD} = (8/15)(8 + e^{2t/5})^{-1}$$

$$\dot{S} = 4\ln[(1 + 2\Delta)/(1 - 2\Delta)]/(15e^{t/5}\sqrt{8 + e^{2t/5}})$$

is it plausible to have nonzero heat and work in an energy-preserving process?

classical example: isothermal process in ideal gasses

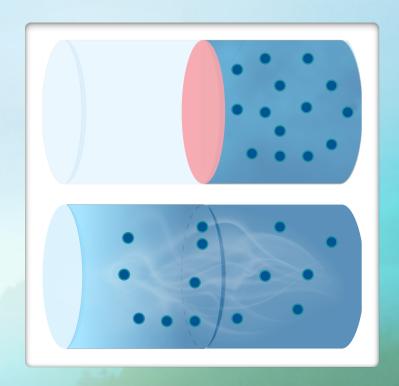


$$\dot{\varrho} = -i[\omega_0 \sigma_z, \varrho] + \gamma (\sigma_z \varrho \sigma_z - \varrho)$$

$$2- |\psi(0)\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$$

$$dU = d\mathbb{Q} = d\mathbb{W}_{CD} = 0$$

$$dS \neq 0$$



classical example: free expansion in ideal gases no heat, no work, only entropy exchange

heat and entropy do not behave monotonically with respect to each other.
is it a discrepancy?!

complete set of orthonormal observables

$$\{O_0 = \mathbb{I}/\sqrt{d} \ , \ O_1 = (1/h)\big(H - \mathrm{Tr}[H]\mathbb{I}/d\big) \ , \ \{O_i\}_{i=2}^{d^2-1} \}$$
 traceless normalized Hamiltonian
$$= \sqrt{\mathrm{Tr}[H^2] - \mathrm{Tr}[H]^2/d}$$

expansion

$$\delta \varrho^{(\text{ev})} = \delta x_1 O_1 + \sum_{i \geqslant 2} \delta x_i O_i$$

independent variables

$$\delta x_1 = \text{Tr}[\delta \varrho^{(\text{ev})} O_1] = \frac{d\mathbb{Q}}{\Delta H}$$

$$\delta x_i = \text{Tr}[\delta \varrho^{(\text{ev})} O_i]$$

$$dS = -\text{Tr}[\delta \varrho^{(\text{ev})} \ln \varrho]$$

$$dS = -\text{Tr}[\delta \varrho^{\text{(ev)}} \ln \varrho] \qquad dS = \frac{\text{Cov}(H, \mathbb{H})}{\Delta^2 H} d\mathbb{Q} + \sum_{i \geqslant 2} \delta x_i \text{Tr}[O_i \mathbb{H}]$$

$$Cov(X,Y) = Tr[(\mathbb{I}/d)XY] - Tr[(\mathbb{I}/d)X]Tr[(\mathbb{I}/d)Y]$$

$$\Delta^2 H = \text{Tr}[(\mathbb{I}/d)H^2] - (\text{Tr}[(\mathbb{I}/d)H])^2$$

$$dS = \frac{\text{Cov}(H, \mathbb{H})}{\Delta^2 H} d\mathbb{Q} + \sum_{i \geqslant 2} \delta x_i \text{Tr}[O_i \mathbb{H}]$$



independent
$$\{d\mathbb{Q}, \{\delta x_i\}_{i=2}^{d^2-1}\}$$

$$\frac{1}{T} = \left(\frac{\partial S}{\partial \mathbb{Q}}\right)_{x_2, x_3, \dots}$$

[arXiv:2105.11915] joint work with F. Benatti, M. Afsary, M. Ramezani, F. Bakhshinezhad, A. T. Rezakhani

entropy production

$$d\Sigma = dS - \frac{d\mathbb{Q}}{T} = \sum_{i \ge 2} \delta x_i \text{Tr}[O_i \mathbb{H}]$$

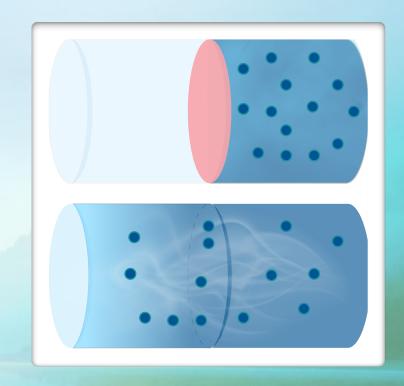
variables of the system other than energy contribute to entropy production

$$\dot{\varrho} = -i[\omega_0 \sigma_z, \varrho] + \gamma (\sigma_z \varrho \sigma_z - \varrho)$$

$$2- |\psi(0)\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$$

$$dU = d\mathbb{Q} = d\mathbb{W}_{CD} = 0$$

$$dS \neq 0$$



$$d\Sigma = dS$$

properties of the presented dynamical and thermodynamic description of quantum Systems:

- fully **geometric** (i.e., trajectory-baed)
- only system-dependent (no need to environment degrees of freedom explicitely)
- entropic-based