Thermalization and 2nd law in closed quantum systems

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Outline

classical energy shell $[E, E+\delta E]$ thermal eq: $p = \dfrac{1}{\mathcal{N}(E)}$

quantum "pure state" $\hat{\rho}^{\psi} = |\psi\rangle\langle\psi|$ & unitary evolution

Macroscopic thermal

macro observable

$$\langle\psi|\hat{M}|\psi\rangle \approx m_{\mathrm{eq}}$$

overwhelming majority

typicality $|\psi\rangle \in \mathbb{S}(\mathcal{H})$

eigenstate thermal. hypo.

$$\langle n|\hat{M}|n\rangle \approx m_{\mathrm{eq}}$$

$$\hat{H}|n\rangle = E_n|n\rangle$$

Microscopic thermal

density operator

subsystem $\hat{\rho}_{\mathrm{s}}^{\psi} = \mathrm{tr}_{\mathrm{B}}\,\hat{\rho}^{\psi}$

thermal $\hat{\rho}_{\mathrm{s}}^{\psi} \approx \mathrm{tr}_{\mathrm{B}}\,\hat{\rho}^{\mathrm{mc}}$

$$\hat{\rho}^{\mathrm{mc}} = \mathrm{d}\,(\mathcal{H})^{-1}\,\hat{P}_{\mathcal{H}}$$

canonical typicality $|\psi\rangle \in \mathbb{S}(\mathcal{H})$

eigenstate thermal. hypo.

$$\hat{\rho}_{\mathrm{s}}^{n} \approx \hat{\rho}_{\mathrm{s}}^{\mathrm{mc}}$$

von Neumann entropy

Classical thermalization

energy shell $[E, E+\delta E]$

phase space

integrable

phase space

non-integrable

thermalize with $p = \dfrac{1}{\mathcal{N}(E)}$

Quantum system

Hilbert space

$$\mathcal{H} = \mathcal{H}_{\rm s} \otimes \mathcal{H}_{\rm B}$$

small huge

Hamiltonian

$$\hat{H} = \hat{H}_{\rm s} + \hat{H}_{\rm B} + \hat{H}_{\rm I}$$ non-integrable

no degeneracy assumed

restricted Hilbert space

$\mathcal{H}_R \subset \mathcal{H}$ spanning $|n\rangle$; $E_n \in [E, E+\delta E]$

$$\hat{H}|n\rangle = E_n|n\rangle$$

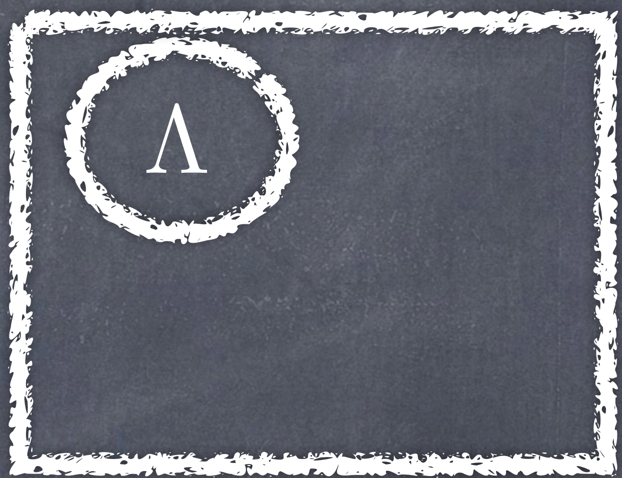
pure state $|\psi\rangle \in \mathbb{S}(\mathcal{H}_R)$

$$|\psi\rangle = \sum_n c_n |n\rangle \qquad |\psi_t\rangle = \sum_n c_n(0) e^{-iE_n t}|n\rangle$$

Equilibrium Hilbert space

von Neumann (1929)

Macroscopic observable on subsystem



$\hat{M}$ energy

magnetization

number density

defined on $\mathcal{H}_R$

spectral decomposition

$$\hat{M} = \sum_{\alpha} m_\alpha |\alpha\rangle\langle\alpha|$$

rounding off

corse-graining

$$\mathcal{H}_R = \bigoplus_{\alpha'} \mathcal{H}_{\alpha'}$$

overwhelming majority $\mathcal{H}_{\mathrm{eq}}$ m_{eq}

$$\mathrm{d}(\mathcal{H}_{\mathrm{eq}})/\mathrm{d}(\mathcal{H}_R) \approx 1$$

example

number density on left

left right

$$m_{\alpha'} = m_0, m_{0.02}, m_{0.04}, \vdots, m_{0.5}, \vdots$$

projection to $\mathcal{H}_{\alpha'}$

$$\hat{P}_{\alpha'} = \sum_{\alpha \in [\alpha' \pm \delta]} |\alpha\rangle\langle\alpha|$$

huge subspace $\mathcal{H}_{\mathrm{eq}}$

Macroscopic thermalization

Goldstein et.al. (2010, 2015)

Definition: if $\langle\psi|\hat{M}|\psi\rangle \approx m_{\rm eq}$ or $\langle\psi|\hat{P}_{\rm eq}|\psi\rangle \approx 1$

pure state $|\psi\rangle \in \mathbb{S}(\mathcal{H}_R)$ is thermal equilibrium

typical pure states $|\psi\rangle \in \mathbb{S}(\mathcal{H}_R)$ thermalize

$$\Big[\langle\psi|\hat{P}_{\rm eq}|\psi\rangle\Big]_\psi = \frac{1}{{\rm d}(\mathcal{H}_R)}{\rm tr}\hat{P}_{\rm eq} = \frac{{\rm d}(\mathcal{H}_{\rm eq})}{{\rm d}(\mathcal{H}_R)} \approx 1$$

uniform average

$${\rm tr}\hat{P}_{\rm eq} = \sum \underbrace{\langle n|\hat{P}_{\rm eq}|n\rangle}_{\approx 1}$$

means $\langle\psi|\hat{P}_{\rm eq}|\psi\rangle \approx 1$ for almost $|\psi\rangle$

even for $|\psi\rangle = |n\rangle$

If initially out of eq.

time average $\overline{\langle\psi_t|\hat{P}_{\rm eq}|\psi_t\rangle} = \sum_n |c_n|^2 \langle n|\hat{P}_{\rm eq}|n\rangle \approx 1$

$\langle\psi_t|\hat{P}_{\rm eq}|\psi_t\rangle \approx 1$

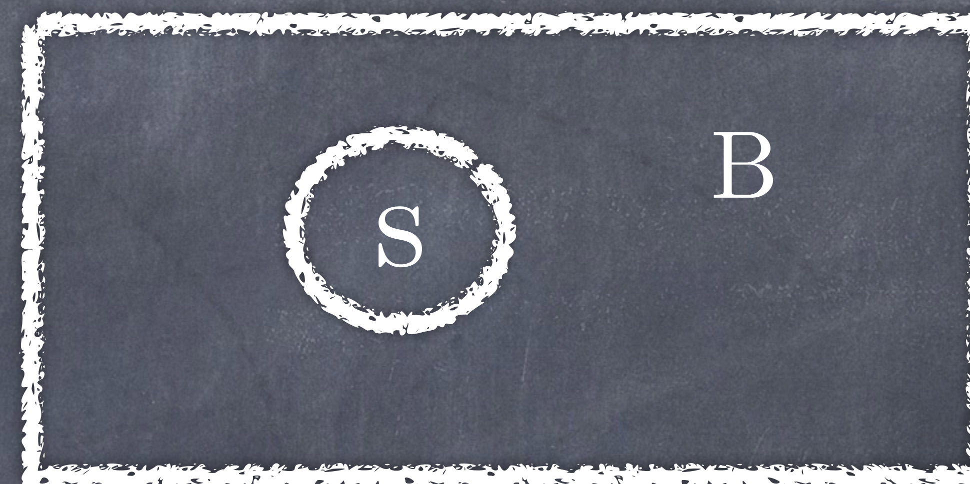
$|\psi_t\rangle = \sum_n c_n e^{-E_n t}|n\rangle$

$\overline{e^{i(E_n - E_{n'})t}} = 0$

thermalizes in long time limit

Macroscopic vs Microscopic

Goldstein et.al. (2015)



pure state $\hat{\rho}^{\psi} = |\psi\rangle\langle\psi|$

$|\psi\rangle \in \mathbb{S}(\mathcal{H}_R)$

macroscopic but local $\hat{M}_{\mathrm{s}}$

on system S

due to overwhelming majority

$$\mathrm{tr}\left\{\hat{M}_{\mathrm{s}}\hat{\rho}^{\psi}\right\} \approx \mathrm{tr}\left\{\hat{M}_{\mathrm{s}}\hat{\rho}^{\mathrm{mc}}\right\} \approx m^{\mathrm{s}}_{\mathrm{eq}}$$ for almost $\hat{\rho}^{\psi}$

$$\hat{\rho}^{\mathrm{mc}} = \frac{\hat{P}_R}{\mathrm{d}(\mathcal{H}_R)}$$

doesnt mean $\hat{\rho}^{\psi} \approx \hat{\rho}^{\mathrm{mc}}$

if $\hat{\rho}^{\psi}_{\mathrm{s}} = \mathrm{tr}_{\mathrm{B}}\,\hat{\rho}^{\psi} \approx \mathrm{tr}_{\mathrm{B}}\,\hat{\rho}^{\mathrm{mc}}$

$$\mathrm{tr}\left\{\hat{M}_{\mathrm{s}}\hat{\rho}^{\psi}\right\} = \mathrm{tr}_{\mathrm{s}}\left\{\hat{M}_{\mathrm{s}}\left(\mathrm{tr}_{\mathrm{B}}\,\hat{\rho}^{\psi}\right)\right\} \approx \mathrm{tr}\left\{\hat{M}_{\mathrm{s}}\hat{\rho}^{\mathrm{mc}}\right\} \approx m^{\mathrm{s}}_{\mathrm{eq}}$$

$\hat{\rho}^{\psi}_{\mathrm{s}} \approx \mathrm{tr}_{\mathrm{B}}\,\hat{\rho}^{\mathrm{mc}}$ means **microscopic** thermalization

Canonical typicality

Popescu et.al. (2006)

random $|\psi\rangle \in \mathbb{S}(\mathcal{H}_R)$ $\quad d_R = \mathrm{d}(\mathcal{H}_R)$ $\; d_\mathrm{s} = \mathrm{d}(\mathcal{H}_\mathrm{s})$ $\; d_\mathrm{B} = \mathrm{d}(\mathcal{H}_\mathrm{B})$

distance between $\hat{\rho}_\mathrm{s}^{\psi} = \mathrm{tr}_\mathrm{B}\, \hat{\rho}^{\psi}$ and $\hat{\rho}_\mathrm{s}^{\mathrm{mc}} = \mathrm{tr}_\mathrm{B}\, \hat{\rho}^{\mathrm{mc}}$

$$D\left(\hat{\rho}_\mathrm{s}^{\psi}, \hat{\rho}_\mathrm{s}^{\mathrm{mc}}\right) = \frac{1}{2}\mathrm{tr}\sqrt{\left(\hat{\rho}_\mathrm{s}^{\psi} - \hat{\rho}_\mathrm{s}^{\mathrm{mc}}\right)^2}$$

levy's lemma

fluctuation with $\epsilon \sim e^{-c\epsilon^2 d_R}$

$$\left[D\left(\hat{\rho}_\mathrm{s}^{\psi}, \hat{\rho}_\mathrm{s}^{\mathrm{mc}}\right)\right]_\psi \leq \frac{1}{2}\sqrt{d_\mathrm{s}/d_\mathrm{B}^{\mathrm{eff}}} \leq \frac{1}{2}\sqrt{d_\mathrm{s}^2/d_R} \sim 0$$

small huge !

effective dim. $d_\mu^{\mathrm{eff}} = \dfrac{1}{\mathrm{tr}\left(\hat{\rho}_\mu^{\mathrm{mc}}\right)^2}$ $\qquad d_R^{\mathrm{eff}} = \dfrac{1}{\mathrm{tr}\left(\hat{\rho}^{\mathrm{mc}}\right)^2} = d_R$

weak subadditivity of Rényi entropy $S_\alpha(\hat{\rho}) = \dfrac{1}{1-\alpha}\ln\left[\mathrm{tr}\hat{\rho}^\alpha\right]$

$$S_\alpha(\hat{\rho}_A) - S_0(\hat{\rho}_B) \leq S_\alpha(\hat{\rho}_{AB}) \leq S_\alpha(\hat{\rho}_A) + S_0(\hat{\rho}_B)$$

A bath
B system
α 2

$$d_R/d_\mathrm{s} \leq d_\mathrm{B}^{\mathrm{eff}} \Longleftarrow \ln\frac{1}{\mathrm{tr}(\hat{\rho}^{\mathrm{mc}})^2} \leq \ln\frac{\mathrm{rank}(\hat{\rho}_\mathrm{s}^{\mathrm{mc}})}{\mathrm{tr}(\hat{\rho}_\mathrm{B}^{\mathrm{mc}})^2}$$

$\mathrm{rank}(\hat{\rho}_\mathrm{s}^{\mathrm{mc}}) \leq d_\mathrm{s}$

Canonical typicality

Goldstein et.al. (2006)

$\mathrm{rank}(\hat{\rho}_{\mathrm{s}}^{\psi}) = \mathrm{rank}(\hat{\rho}_{\mathrm{B}}^{\psi}) \leq d_{\mathrm{s}}$

Canonical typicality

bath is not thermal $\hat{\rho}_{\mathrm{B}}^{\psi} \not\approx \hat{\rho}_{\mathrm{B}}^{\mathrm{mc}}$

$$\hat{\rho}_{\mathrm{s}}^{\psi} = \mathrm{tr}_{\mathrm{B}}\, \hat{\rho}^{\psi} \approx \mathrm{tr}_{\mathrm{B}}\, \hat{\rho}^{\mathrm{mc}}$$

almost all pure states $d_R \gg 1$

small d_{s}

weak interaction limit $||\hat{H}_{\mathrm{I}}|| \ll 1$

$$|\Phi\rangle = \sum_{ij} c_{ij} |\mathrm{s}_i\rangle|\mathrm{B}_j\rangle \qquad |\psi\rangle = \frac{|\Phi\rangle}{\sqrt{\langle\Phi|\Phi\rangle}}$$

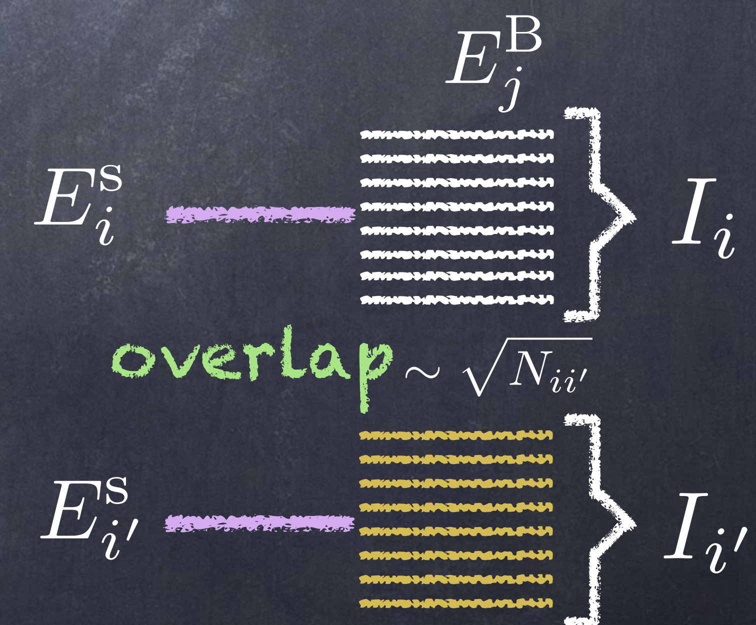
energy eigenstates

with normalization

gaussian random

$\hat{H}_{\mathrm{s}}$ $\hat{H}_{\mathrm{B}}$

$c_{ij} \neq 0$ $\quad E_i^{\mathrm{s}} + E_j^{\mathrm{B}} \in [E, E + \delta E]$



partial trace

$|\Phi_i\rangle = \sum_{j\in I_i} c_{ij}|B_j\rangle$

$$\mathrm{tr}_{\mathrm{B}}|\psi\rangle\langle\psi| = \frac{1}{\langle\Phi|\Phi\rangle}\sum_{ii'} \mathrm{tr}_{\mathrm{B}}\, |\Phi_i\rangle\langle\Phi_{i'}| \otimes |\mathrm{s}_i\rangle\langle\mathrm{s}_{i'}|$$

$$= \langle\Phi_i|\Phi_{i'}\rangle \approx \delta_{ii'} N_i$$

$$\approx \frac{1}{d_R}\sum_i N_i |\mathrm{s}_i\rangle\langle\mathrm{s}_i| = \mathrm{tr}_{\mathrm{B}}\, \hat{\rho}^{\mathrm{mc}} = \mathrm{tr}_{\mathrm{B}} (1/d_R) \sum_{ij} |\mathrm{s}_i\rangle\langle\mathrm{s}_i| \otimes |\mathrm{B}_j\rangle\langle\mathrm{B}_j|$$

Equilibration

Linden et.al. (2009)

$|\psi_0\rangle = |\phi_{\rm s}\rangle \otimes |\phi_{\rm B}\rangle$

Although pure states are not thermal eq. initially,

almost $|\psi_t\rangle = \sum_n c_n e^{-E_n t}|n\rangle$ will be thermal in long time:

time averaged

$\hat{\omega}^{\psi} = \overline{\hat{\rho}^{\psi_t}} = \sum_n |c_n|^2 |n\rangle\langle n|$ assuming nondegeneracy

distance between $\hat{\rho}_{\rm s}^{\psi_t}$ and $\hat{\omega}_{\rm s}^{\psi} = {\rm tr_B}\,\hat{\omega}^{\psi}$

$$D\left(\hat{\rho}_{\rm s}^{\psi_t}, \hat{\omega}_{\rm s}^{\psi}\right) = \frac{1}{2}{\rm tr}\sqrt{\left(\hat{\rho}_{\rm s}^{\psi_t} - \hat{\omega}_{\rm s}^{\psi}\right)^2} \qquad d^{\rm eff}(\hat{\omega}_{\mu}^{\psi}) = \frac{1}{{\rm tr}(\hat{\omega}_{\mu}^{\psi})^2} \qquad d^{\rm eff}(\hat{\omega}^{\psi}) > d_R/4$$

$$\overline{D\left(\hat{\rho}_{\rm s}^{\psi_t}, \hat{\omega}_{\rm s}^{\psi}\right)} \le \frac{1}{2}\sqrt{d_{\rm s}/d^{\rm eff}(\hat{\omega}_{\rm B}^{\psi})} \le \frac{1}{2}\sqrt{d_{\rm s}^2/d^{\rm eff}(\hat{\omega}^{\psi})} \sim 0$$

small

huge !

weak subadditivity
of Rényi entropy

fluctuation with ϵ

$\sim e^{-c'\epsilon^4 d^{\rm eff}(\hat{\omega}^{\psi})}$

Levy's lemma

Therefore $\hat{\rho}_{\rm s}^{\psi_t} \approx \hat{\omega}_{\rm s}^{\psi} \approx \hat{\rho}_{\rm s}^{\rm mc}$ i.c. independent typicality

Eigenstate thermalization hypothesis

Goldstein et.al. (2015)

A single (atypical) eigenstate is thermal equilibrium?

recall macro thermalization

$$\frac{1}{d_R}\mathrm{tr}\,\hat{P}_{\mathrm{eq}} = \frac{1}{d_R}\sum_n \langle n|\hat{P}_{\mathrm{eq}}|n\rangle = \frac{\mathrm{d}(\mathcal{H}_{\mathrm{eq}})}{d_R} \approx 1 \longrightarrow \langle n|\hat{P}_{\mathrm{eq}}|n\rangle \approx 1$$

ETH !

$$\langle n|\hat{M}|n\rangle \approx m_{\mathrm{eq}}$$

energy eigenstate $|n\rangle$

overwhelming majority

Microscopic ETH

let $|\psi\rangle = |n\rangle$ $\mathrm{tr}_{\mathrm{B}}(\hat{\rho}^n = |n\rangle\langle n|)$ ETH means $\hat{\rho}^n_{\mathrm{s}} \approx \hat{\rho}^{\mathrm{mc}}_{\mathrm{s}}$

numerically supported

e.x.) $\hat{H} = \sum_i h_i \hat{\sigma}^z_i + \sum_{ij} J_{ij}\hat{\sigma}_i \cdot \hat{\sigma}_j$

ETH not always holds

Many body localization ← strong disorder

Nandkishore & Huse (2015)

$J_{ij} \to 0$ $|\psi\rangle = |\sigma^z_1\rangle \otimes |\sigma^z_2\rangle \otimes \cdots$

Macro vs Micro ETH

Goldstein et.al. (2015)

microscopic

Even though eigenstates with MBL do not thermalize,

macroscopic thermalization

$$\frac{1}{d_R}\mathrm{tr}\,\hat{P}_{\mathrm{eq}} = \frac{1}{d_R}\sum_n \langle n|\hat{P}_{\mathrm{eq}}|n\rangle = \frac{\mathrm{d}(\mathcal{H}_{\mathrm{eq}})}{d_R} \approx 1 \longrightarrow \langle n|\hat{P}_{\mathrm{eq}}|n\rangle \approx 1$$

energy eigenstate $|n\rangle$

nothing to do with destiny operator

system with MBL $\hat{H} = \sum_i h_i \hat{\sigma}_i^z + \sum_{ij} J_{ij}\hat{\sigma}_i \cdot \hat{\sigma}_j$ random h_i

$J_{ij} \to 0$ eigenstate has a form $|n\rangle = |\sigma_1^z\rangle \otimes |\sigma_1^z\rangle \otimes \cdots$

$\hat{\rho}_{\mathrm{s}}^n \not\approx \hat{\rho}_{\mathrm{s}}^{\mathrm{mc}}$

measuring magnetization on S within energy shell

almost all $\langle n|\hat{M}_{\mathrm{s}}|n\rangle \approx m_{\mathrm{eq}}^{\mathrm{s}}$ overwhelming majority

Macro th. eq. does not mean micro th. eq.

Entropy in a closed system

Hamiltonian system

Liouville theorem works

classical closed system

system entropy = Shannon entropy

$$H = -\sum_i p_i \ln p_i$$

"System entropy is invariant for time evolution"

quantum corresponding

von Neumann entropy $S(\hat{\rho}) = -\mathrm{tr}\,\hat{\rho}\ln\hat{\rho}$

for pure states $S(|\psi\rangle\langle\psi|) = 0$

entropy change in closed quantum system

$$\Delta S = S(\hat{\rho}_{t_2}) - S(\hat{\rho}_{t_1}) = 0$$ trivial!

$\hat{\rho}_{t_2} = \hat{U}(t_2;t_1)\hat{\rho}_{t_1}\hat{U}^\dagger(t_2;t_1)$ unitary evolution

Subsystem decomposition

Esposito et.al. (2010); Sagawa (2014)

bipartite quantum system

general situation

$\hat{\rho}_{AB}$

$$\hat{\rho}_A = \mathrm{tr}_B\, \hat{\rho}_{AB}$$
$$\hat{\rho}_B = \mathrm{tr}_A\, \hat{\rho}_{AB}$$

initially, $\hat{\rho}_{AB}(0) = \hat{\rho}_A(0) \otimes \hat{\rho}_B(0)$ $\quad S[\hat{\rho}(t)] = -\mathrm{tr}[\hat{\rho}(t) \ln \hat{\rho}(t)]$

$$S[\hat{\rho}_{AB}(0)] = S[\hat{\rho}_A(0)] + S[\hat{\rho}_B(0)]$$

at time t $\hat{\rho}_{AB}(t) \neq \hat{\rho}_A(t) \otimes \hat{\rho}_B(t)$ → not additive $S[\hat{\rho}_{AB}(t)]$

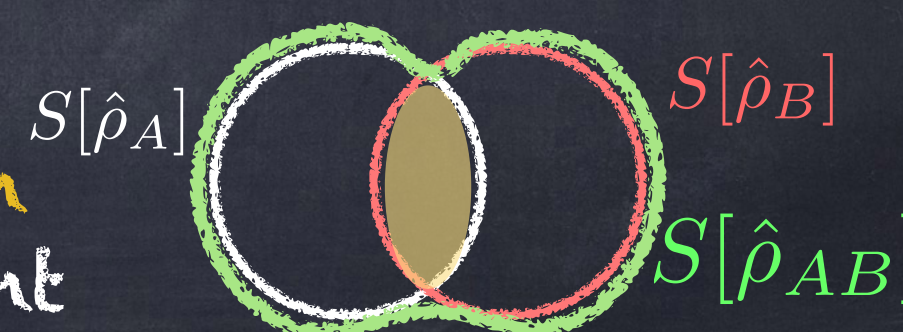
positive entropy production

$$S[\hat{\rho}_A(t)] + S[\hat{\rho}_B(t)] - S[\hat{\rho}_{AB}(0)] = S[\hat{\rho}_A(t)] + S[\hat{\rho}_B(t)] - S[\hat{\rho}_{AB}(t)]$$

$$\Delta S_A + \Delta S_B = I_{\mathrm{Q}}(t) \geq 0$$

quantum mutual information

pure state $\Delta S_A = \Delta S_B$ entanglement



Canonical heat bath

Esposito et.al. (2010); Sagawa (2014)

If initial bath $\hat{\rho}_{\mathrm{B}}(0) = e^{-\beta \hat{H}_{\mathrm{B}}}/Z_{\mathrm{B}}$

$$\hat{\rho}_{\mathrm{sB}}(0) = \hat{\rho}_{\mathrm{s}}(0) \otimes \hat{\rho}_{\mathrm{B}}(0)$$

$$S[\hat{\rho}(t)] = -\mathrm{tr}[\hat{\rho}(t) \ln \hat{\rho}(t)]$$

$$-S[\hat{\rho}_{\mathrm{sB}}(0)] = -S[\hat{\rho}_{\mathrm{sB}}(t)]$$

$$\|$$

$$-\left(S[\hat{\rho}_{\mathrm{s}}(0)] + \beta \mathrm{tr}\left[\hat{\rho}_{\mathrm{B}}(0)\hat{H}_{\mathrm{B}}\right] + \ln Z_{\mathrm{B}}\right)$$

$$S[\hat{\rho}_{\mathrm{s}}(t)] + \beta \mathrm{tr}\left[\hat{\rho}_{\mathrm{B}}(t)\hat{H}_{\mathrm{B}}\right] + \ln Z_{\mathrm{B}}$$

energy change in bath Q

quantum relative entropy

positive !

$$\Delta S_{\mathrm{s}} + \beta Q = \mathrm{tr}\left[\hat{\rho}_{\mathrm{sB}}(t) \ln \frac{\hat{\rho}_{\mathrm{sB}}(t)}{\hat{\rho}_{\mathrm{s}}(t) \otimes \hat{\rho}_{\mathrm{B}}(0)}\right] \geq 0$$

c.f.) general form initially product state

$$\Delta S_{\mathrm{s}} + \Delta S_{\mathrm{B}} = I_{\mathrm{Q}}(\mathrm{s} : \mathrm{B}) \geq 0$$

entropy change in bath

quantum mutual info.

Pure state heat bath

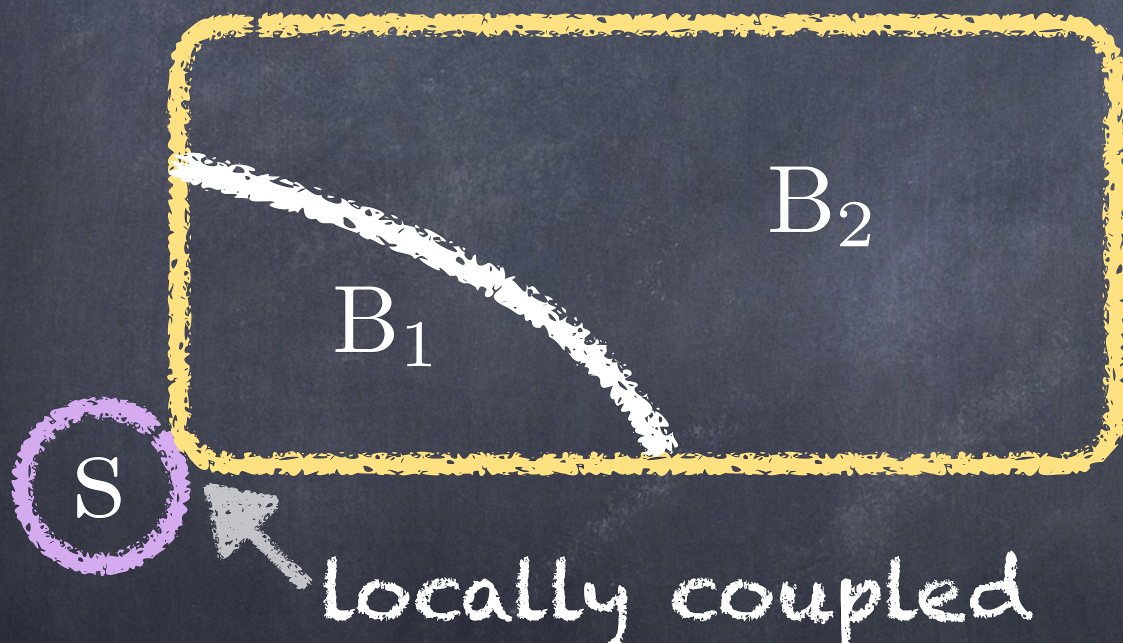
Iyoda et.al. (2016)

typical $d_{\mathrm{B}} \gg 1$

If initial bath $\hat{\rho}_{\mathrm{B}}(0) = |\phi_{\mathrm{B}}\rangle\langle\phi_{\mathrm{B}}|$ $\hat{\rho}_{\mathrm{sB}}(0) = \hat{\rho}_{\mathrm{s}}(0) \otimes \hat{\rho}_{\mathrm{B}}(0)$

$\Delta S_{\mathrm{s}} + \Delta S_{\mathrm{B}} \geq 0$ ok!, but $\Delta S_{\mathrm{s}} + \beta Q \geq 0$? yes

at the beginning



macroscopic

$d_{\mathrm{B}} \gg d_{\mathrm{B}_1}$

$$\hat{\rho}_{\mathrm{B}_1} \approx \mathrm{tr}_{\mathrm{B}_2} \hat{\rho}_{\mathrm{B}}^{\mathrm{mc}}$$

$$\approx e^{-\beta \hat{H}_{\mathrm{B}_1}} / Z_{\mathrm{B}_1}$$

weak int. between B_1 & B_2

Effectively system feels canonical bath $e^{-\beta \hat{H}_{\mathrm{B}_1}} / Z_{\mathrm{B}_1}$

until it is aware of the reminder B_2

not thermal density op.

Summary

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$$\hat{\rho}^{\mathrm{mc}} = \mathrm{d}\,(\mathcal{H})^{-1}\, \hat{P}_{\mathcal{H}}$$

canonical typicality $|\psi\rangle \in \mathbb{S}(\mathcal{H})$

eigenstate thermal. hypo.

$$\hat{\rho}^{n}_{\mathrm{s}} \approx \hat{\rho}^{\mathrm{mc}}_{\mathrm{s}}$$

von Neumann entropy

$$\Delta S_{\mathrm{s}} + \beta Q \geq 0$$