Correlations in thermodynamics of quantum systems beyond the weak-coupling regime

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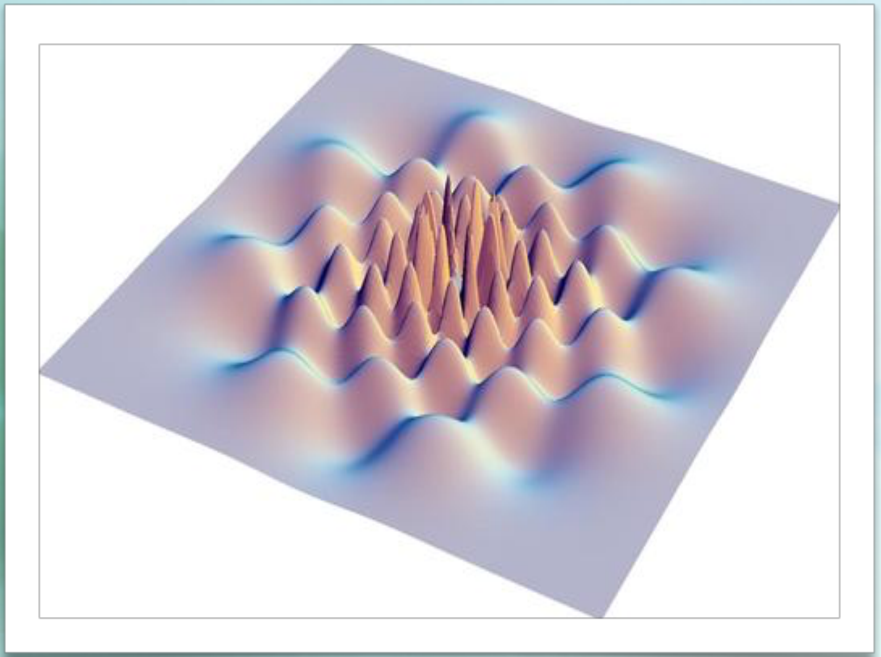
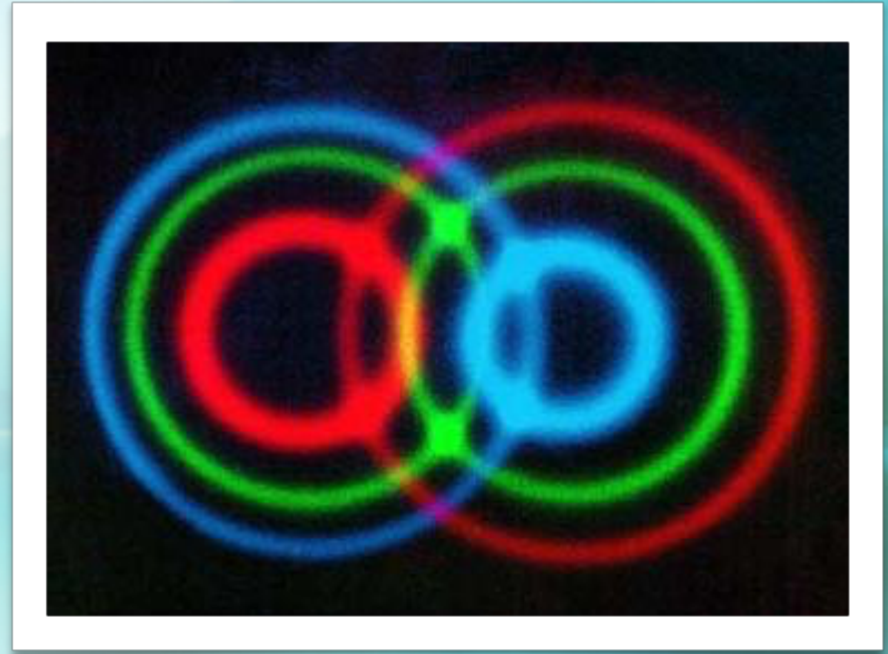
One of the main goals in q. thermodynamics: using q. features in thermodynamic processes



superposition / coherence



quantum correlations (entanglement)

PHYSICAL REVIEW B 90, 075421 (2014)

Heat due to system-reservoir correlations in thermal equilibrium

Joachim Ankerhold[1,*] and Jukka P. Pekola[2]

arXiv:1510.05035v2 [quant-ph] 16 Oct 2017

No energy transport without discord

Seth Lloyd,[1,2] Zi-Wen Liu,[3,2] Stefano Pirandola,[4] Vazrik Chiloyan,[1] Yongjie Hu,[5] Samuel Huberman,[1] and Gang Chen[1]

PHYSICAL REVIEW X 5, 041011 (2015)

Extractable Work from Correlations

Martí Perarnau-Llobet,[1] Karen V. Hovhannisyan,[1] Marcus Huber,[2,1] Paul Skrzypczyk, Nicolas Brunner,[4] and Antonio Acín[1,5]

nature COMMUNICATIONS 2017

ARTICLE

DOI: 10.1038/s41467-017-02370-x OPEN

Generalized laws of thermodynamics in the presence of correlations

Manabendra N. Bera[1,2], Arnau Riera[1,2], Maciej Lewenstein[1,3] & Andreas Winter[3,4]

https://doi.org/10.1038/s41467-019-10333-7

nature COMMUNICATIONS 2019

ARTICLE

https://doi.org/10.1038/s41467-019-10333-7 OPEN

Reversing the direction of heat flow using quantum correlations

Kaonan Micadei[1,2,8], John P.S. Peterson[3,8], Alexandre M. Souza[3], Roberto S. Sarthour[3], Ivan S. Oliveira[3], Gabriel T. Landi[4], Tiago B. Batalhão[5,6], Roberto M. Serra[1,7] & Eric Lutz[2]

ONS 2019

41467-019-10572

PHYSICAL REVIEW LETTERS 122, 047702 (2019)

Extractable Work, the Role of Correlations, and Asymptotic Freedom in Quantum Batteries

Gian Marcello Andolina,[1,2] Maximilian Keck,[3] Andrea Mari,[3] Michele Campisi,[4,5] Vittorio Giovannetti,[3] and Marco Polini[1]

Correlations as a resource in quantum thermodynamics

Facundo Sapienza[1], Federico Cerisola[1,2] & Augusto J. Roncaglia[1,2]

strong coupling

↓

non-Markovinaity

↕

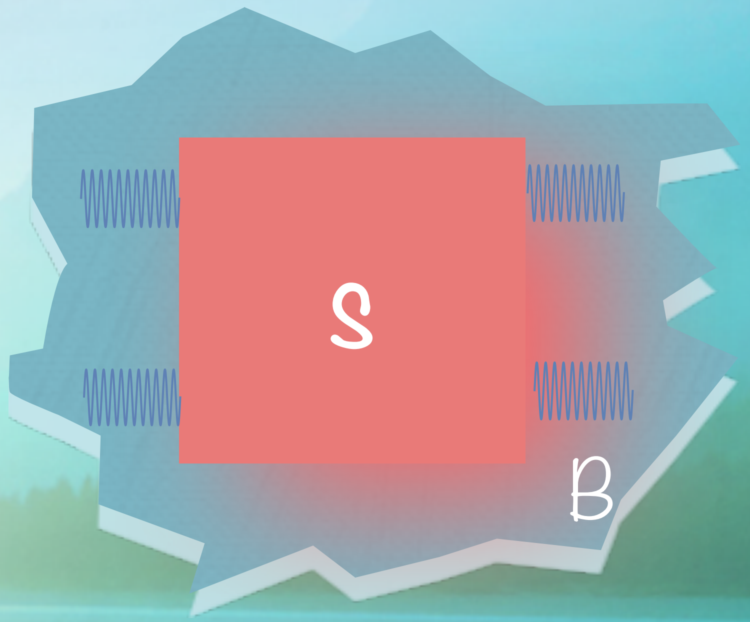
correlation

a general framework to take into account correlation

— a thermodynamic system is an **open** system, i.e., in **interaction** with a bath

interaction

Energy is not additive with respect to bare Hamiltonians



$$H_{\mathsf{SB}} = H_{\mathsf{S}} + H_{\mathsf{B}} + H_{\mathrm{I}}$$

a fundamental issue about interacting systems: **subsystem Hamiltonian?**

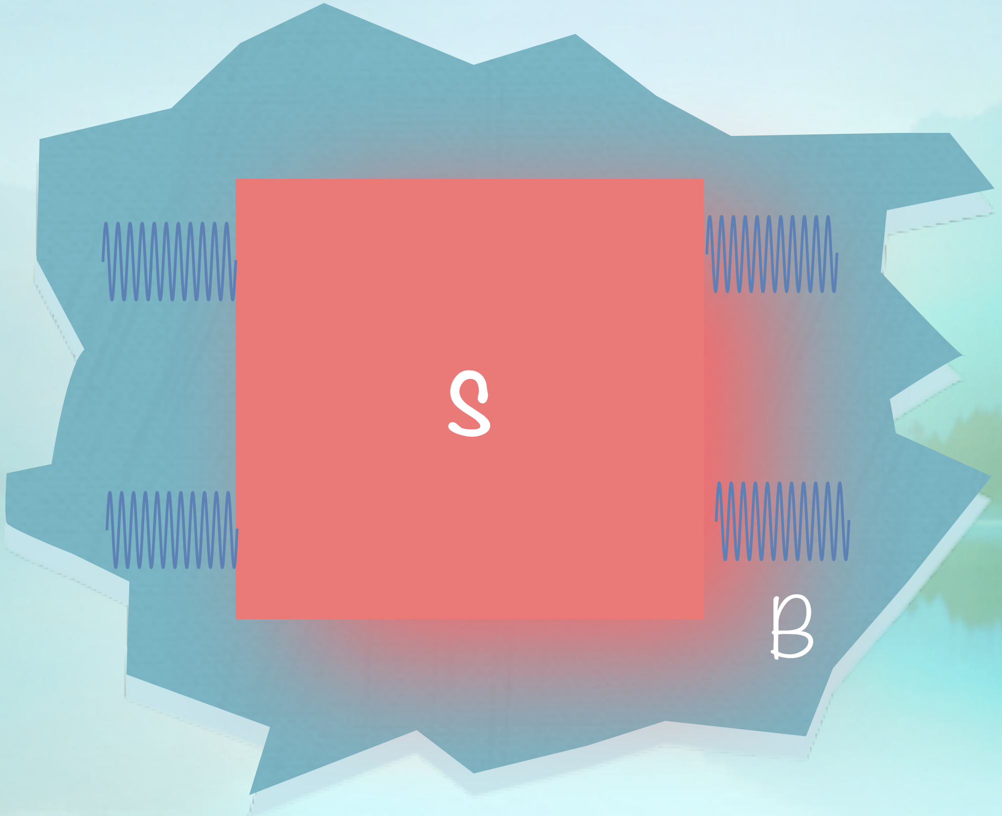
Back to the origin of “Hamiltonian”:

it came into play when describing **dynamics:**

$$\dot{p} = -\frac{\partial H}{\partial q} \qquad \dot{q} = \frac{\partial H}{\partial p}$$

to define subsystem Hamiltonian $\longrightarrow$ subsystem dynamics

A postulate of quantum mechanics: Closed system evolves unitarily

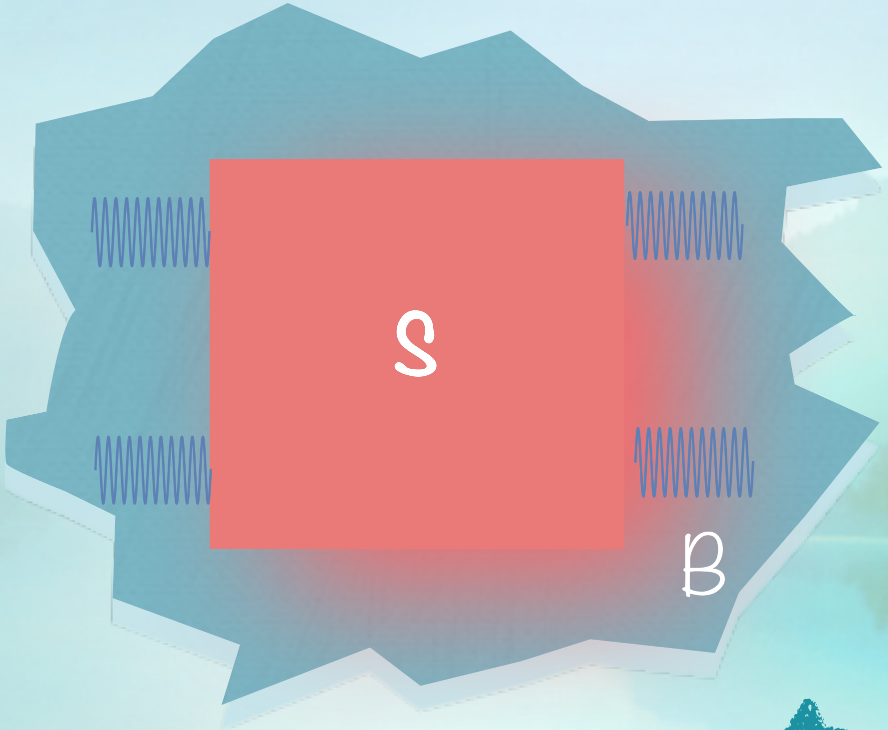


$$H_{\mathsf{SB}} = H_{\mathsf{S}} + H_{\mathsf{B}} + H_{\mathrm{I}}$$

$$\dot{\varrho}_{\mathsf{SB}}(\tau) = -i[H_{\mathsf{SB}}, \varrho_{\mathsf{SB}}]$$

What about the system alone?

$$\varrho_{SB} \neq \varrho_S \otimes \varrho_B$$



$$\varrho_{SB} = \varrho_S \otimes \varrho_B + \chi$$

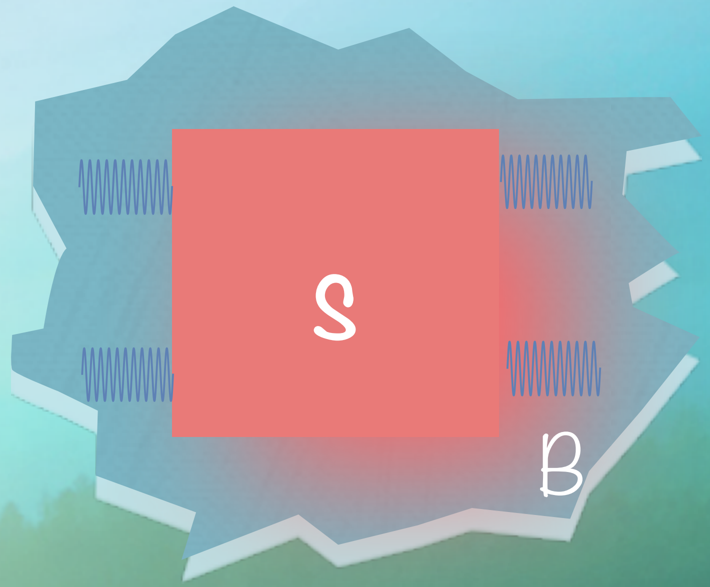
correlation

$$\mathrm{Tr}_S[\chi] = \mathrm{Tr}_B[\chi] = 0$$

dynamics of open quantum system (**time independent** total Hamiltonian):

$$\varrho_{\mathrm{SB}}(\tau) = \varrho_{\mathrm{S}}(\tau) \otimes \varrho_{\mathrm{B}}(\tau) + \chi(\tau)$$

$$\dot{\varrho}_S(\tau) = -i\,\mathrm{Tr}_B[H_{SB}, \varrho_{SB}(\tau)]$$

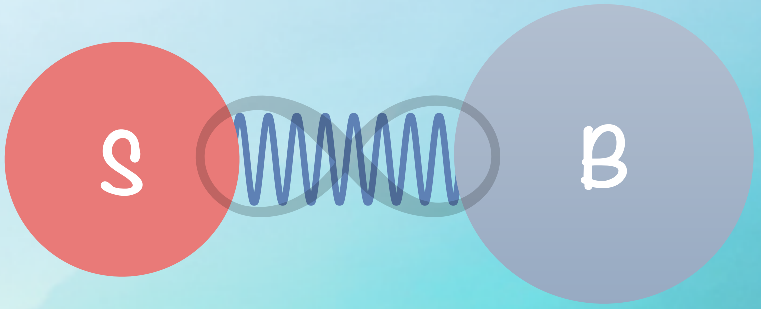


$$\dot{\varrho}_S(\tau) = \underbrace{\boxed{-i[H'_S(\tau), \varrho_S(\tau)]}}_{\text{coherent}} - \underbrace{\boxed{i\,\mathrm{Tr}_B[H_{\mathrm{I}}, \chi(\tau)]}}_{\text{incoherent}}$$

$$H'_S = H_S + \underbrace{\boxed{\mathrm{Tr}_B[H_{\mathrm{I}}\varrho_B]}}_{\text{environment-induced correction}} \longrightarrow H_S^{(\mathrm{eff})}(\tau)$$

a **freedom** in definition of subsystem Hamiltonian: $H_S^{(\mathrm{eff})}(\tau)$

$$H_{\mathrm{I}}^{(\mathrm{eff})}(\tau) = H_{SB} - H_S^{(\mathrm{eff})}(\tau) - H_B^{(\mathrm{eff})}(\tau)$$



using the freedom: $\boxed{\mathrm{Tr}_S[\varrho_S\, H_{\mathrm{I}}^{(\mathrm{eff})}] = \mathrm{Tr}_B[\varrho_B\, H_{\mathrm{I}}^{(\mathrm{eff})}] = 0}$

interaction energy **inaccessible** through either of subsystems

$$\boxed{\begin{aligned} H_S^{\mathrm{eff}}(\tau) &= H'_S(\tau) - \alpha_S \mathrm{Tr}[\varrho_S(\tau) \otimes \varrho_B(\tau) H_{\mathrm{I}}] \\ H_B^{\mathrm{eff}}(\tau) &= H'_B(\tau) - \alpha_B \mathrm{Tr}[\varrho_S(\tau) \otimes \varrho_B(\tau) H_{\mathrm{I}}] \end{aligned}}$$

$$\alpha_S + \alpha_B = 1$$

$\boxed{\mathbb{U}_\chi(\tau) = \mathrm{Tr}[\chi(\tau)\, H_{\mathrm{I}}^{(\mathrm{eff})}]}$ **binding energy**: an energy associated to **correlation**

correlation

interaction

$$\boxed{\mathbb{U}_{\mathrm{tot}} = \mathbb{U}_S(\tau) + \mathbb{U}_B(\tau) + \mathbb{U}_\chi(\tau)}$$

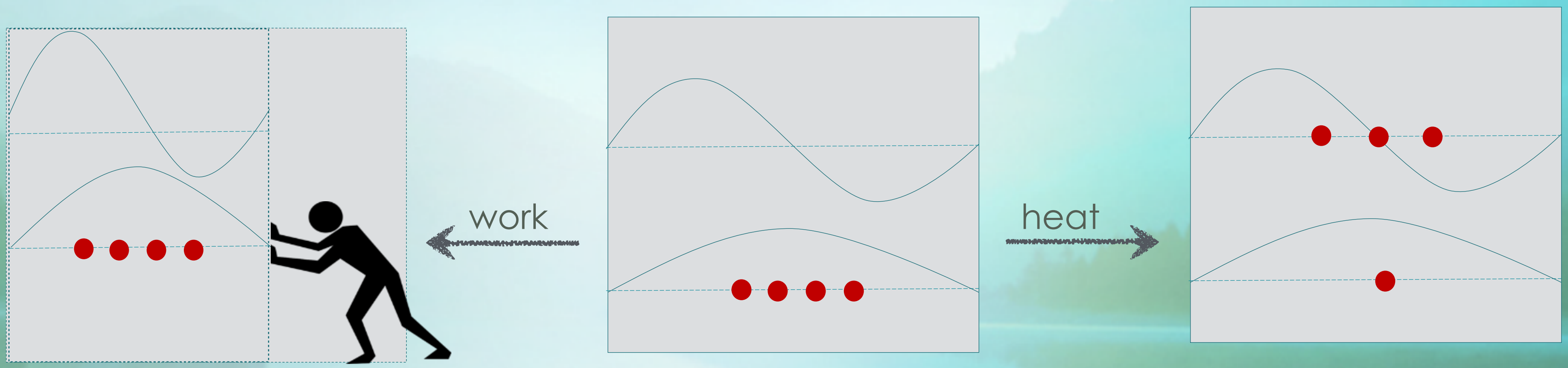
non-additive
non-extensive

energy change due to change in H

energy change due to change in the state

$$\mathrm{d}\mathbb{W}(\tau) = \mathrm{Tr}[\varrho(\tau)\,\mathrm{d}H^{(\mathrm{eff})}(\tau)]$$

$$\mathrm{d}\mathbb{Q}(\tau) = \mathrm{Tr}[\mathrm{d}\varrho(\tau)\,H^{(\mathrm{eff})}(\tau)]$$



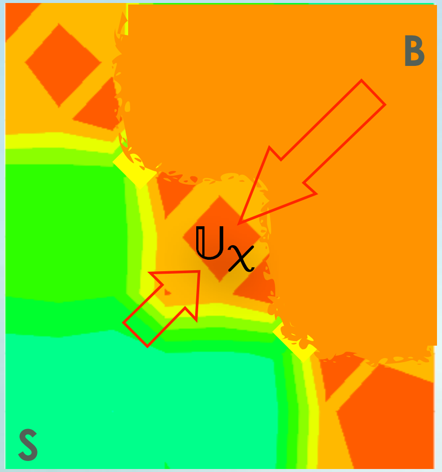
energy levels

population

1st law of thermodynamics

$$\boxed{\mathrm{d}\mathbb{U} = \mathrm{d}\mathbb{Q} + \mathrm{d}\mathbb{W}}$$

—correlation in work/heat exchange:



$$\mathrm{d}\mathbb{U}_S(\tau) + \mathrm{d}\mathbb{U}_B(\tau) = -\mathrm{d}\mathbb{U}_\chi(\tau) \qquad \mathrm{d}\mathbb{U}_\chi = \mathrm{Tr}[\mathrm{d}\chi H_{\mathrm{int}}]$$

energy conservation relation

$$\boxed{\begin{aligned} \mathrm{d}\mathbb{W}_S(\tau) + \mathrm{d}\mathbb{W}_B(\tau) &= 0 \\ \mathrm{d}\mathbb{Q}_S(\tau) + \mathrm{d}\mathbb{Q}_B(\tau) &= -\mathrm{d}\mathbb{U}_\chi(\tau) \end{aligned}}$$

—manifestation of Newton's 3rd law (action-reaction)

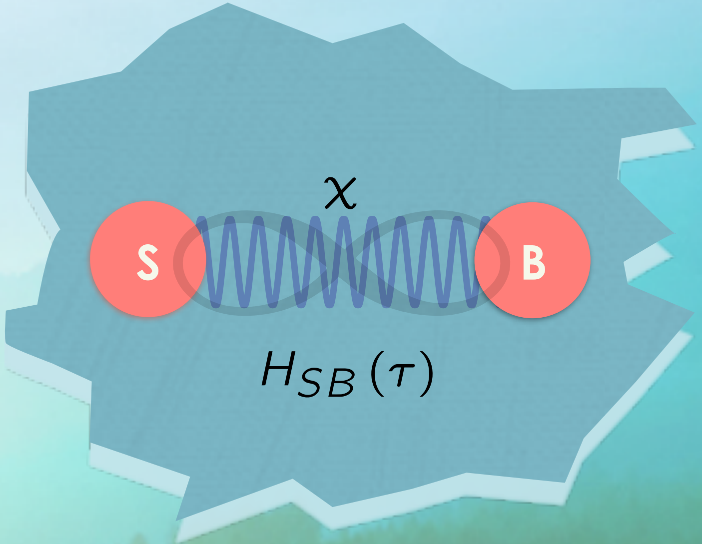
—correlations may be a source/storage for heat

—heat exchange may yield correlations

[SA, Benatti, Bakhshinezhad, Afsary, Marcantoni, Rezakhani, Sci. Rep. (2016)]

what if the the total system is open and Hamiltonian is time dependent?

$$\dot{\varrho}_{\mathrm{SB}}(\tau) = -i[H_{\mathrm{SB}}(\tau), \varrho_{\mathrm{SB}}(\tau)] + \mathcal{L}[\varrho_{\mathrm{SB}}(\tau)]$$



$$\boxed{\begin{aligned} \mathrm{d}\mathbb{W}_{SB} &= \mathrm{d}\mathbb{W}_S + \mathrm{d}\mathbb{W}_B + \mathrm{d}\mathbb{W}_\chi \\ \mathrm{d}\mathbb{Q}_{SB} &= \mathrm{d}\mathbb{Q}_S + \mathrm{d}\mathbb{Q}_B + \mathrm{d}\mathbb{Q}_\chi \end{aligned}}$$

— Markovian environmnet
— System is driven

$$\mathrm{d}\mathbb{W}_{SB} = \mathrm{Tr}[\varrho_{SB}\ \mathrm{d}H_{SB}]$$

$$\mathrm{d}\mathbb{Q}_{SB} = \mathrm{Tr}[\mathrm{d}\varrho_{SB}\ H_{SB}]$$

$$\mathrm{d}\mathbb{W}_\chi = \mathrm{Tr}[\chi\ \mathrm{d}H_{\mathrm{int}}]$$

$$\mathrm{d}\mathbb{Q}_\chi = \mathrm{Tr}[\mathrm{d}\chi\ H_{\mathrm{int}}]$$

what if the the total system is open and Hamiltonian is time dependent?

- if $d\mathbb{W}_S = d\mathbb{W}_B = 0$ $\longrightarrow$ extraction of **work** from **correlation** $d\mathbb{W}_{SB} = -d\mathbb{W}_\chi$

  Perarnau-Llobet *et al.*, PRX(2015)

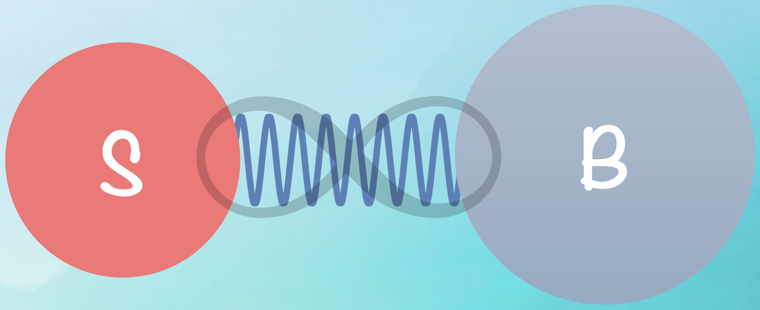
- if $d\mathbb{Q}_S = d\mathbb{Q}_B = 0$ $\longrightarrow$ conversion of **external heat** to **correlation** $d\mathbb{Q}_{SB} = -d\mathbb{Q}_\chi$

  Ankerhold & Pekola, PRB (2014)

- if $d\mathbb{Q}_{SB} = d\mathbb{Q}_B = 0$ $\longrightarrow$ conversion of **system heat** to **correlation** $d\mathbb{Q}_S = -d\mathbb{Q}_\chi$ Lloyd et al. arXiv:1510.05035

  local correlation witness

—entropy in closed combined systems:



$$\$(\tau) = -\mathrm{Tr}[\varrho(\tau)\log\varrho(\tau)]$$

sum of subsystem entropies $\neq$ total entropy

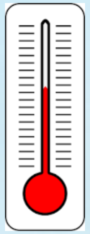
mutual information $\$_\chi(\tau) = \$_S(\tau) + \$_B(\tau) - \$_{SB}(\tau) \geqslant 0$

closed composite system: **constant** total entropy $\longrightarrow$ $d\$_S(\tau) + d\$_B(\tau) = d\$_\chi(\tau)$

a manifestation of 2nd law of thermodynamics:

$\$_\chi(0) = 0$ $\longrightarrow$ $\boxed{\Delta\$_S(\tau) + \Delta\$_B(\tau) = \$_\chi(\tau) \geqslant 0}$

—how about "temperature"?



standard thermodynamic definition $1/T := (\partial\mathbb{S}/\partial\mathbb{U})_{N,V,\ldots}$

pseudo-temperature: $1/T(\tau) := \mathrm{d}\mathbb{S}(\tau)/\mathrm{d}\mathbb{U}(\tau)$

pseudo-temperature for correlation: $1/T_\chi(\tau) = \mathrm{d}\mathbb{S}_\chi/\mathrm{d}\mathbb{U}_\chi$

entropy change relation in a closed system

$$\mathrm{d}\mathbb{S}_S(\tau) + \mathrm{d}\mathbb{S}_B(\tau) = \mathrm{d}\mathbb{S}_\chi(\tau) \longleftrightarrow \mathrm{d}\mathbb{U}_S/T_S + \mathrm{d}\mathbb{U}_B/T_B = \mathrm{d}\mathbb{U}_\chi/T_\chi$$

$$\boxed{\begin{matrix} \mathrm{d}\mathbb{U}_\chi = 0 \\ T_\chi \neq 0 \end{matrix} \Rightarrow T_S = T_B \text{ thermal equilibrium}}$$

(zeroth law of thermodynamics)

—a better way to define temperature:

recall
$$\mathrm{d}\mathbb{S}_S = \mathrm{d}\mathbb{Q}_S/T + \mathrm{d}\Sigma_S$$

temperature and internal entropy production are unknown

uniquely determine temperature?

—a systematic approach:

a set of relevant physical observables (orthonormal and traceless) $\mathcal{A} = \{A_i\}_{i=1}^{d_S^2-1}$

$$A_0 = \mathbb{I}/\sqrt{d_S}$$

system Hamiltonian

$$A_1 = (1/h)\Big(H - \mathrm{Tr}[H]\,\mathbb{I}/d_S\Big)$$

normalization factor $h = \sqrt{\mathrm{Tr}[A_1^2]}$

$$\ldots$$

coordinates: $\mathrm{x}_i(\tau) = \mathrm{Tr}[\varrho(\tau)\,A_i(\tau)], \quad i \in \{0, 1, \ldots, d_S^2 - 1\}$

$$\varrho(\{\mathrm{x}_i\};\tau) = \sum_{i=0}^{d_S^2-1} \mathrm{x}_i(\tau) A_i(\tau)$$

$$\mathrm{d}\varrho(\{\mathrm{y}_i\};\tau) = \sum_{i>0} \mathrm{dy}_i\, A_i$$

not exact differentials

$$\mathrm{d}\mathbb{Q}(\{\mathrm{y}_i\}) = \mathrm{Tr}[\mathrm{d}\varrho\, H] = h\,\boxed{\mathrm{dy}_1}$$

$$\mathrm{d}\mathbb{S}(\{\mathrm{y}_i\};\tau) = -\sum_{i>0} \mathrm{Tr}[A_i \log\varrho]\ \mathrm{dy}_i \longrightarrow \mathrm{d}\mathbb{S}(\{\mathrm{y}_i\}) = \frac{1}{\mathcal{T}}\,\mathrm{d}\mathbb{Q} - \sum_{i\neq 0,1} \mathrm{Tr}[A_i \log\varrho]\,\mathrm{dy}_i$$

$$\Rightarrow \boxed{\frac{1}{\mathcal{T}} = -\frac{\mathrm{Cov}(H, H_{\mathrm{ent}})}{\Delta^2 H}}$$

where

$$H_{\mathrm{ent}} := -\boxed{\log\varrho} - \log Z$$

$$\mathrm{Cov}(X, Y) := \mathrm{Tr}[XY]/d_S - \mathrm{Tr}[X]\mathrm{Tr}[Y]/d_S^2$$

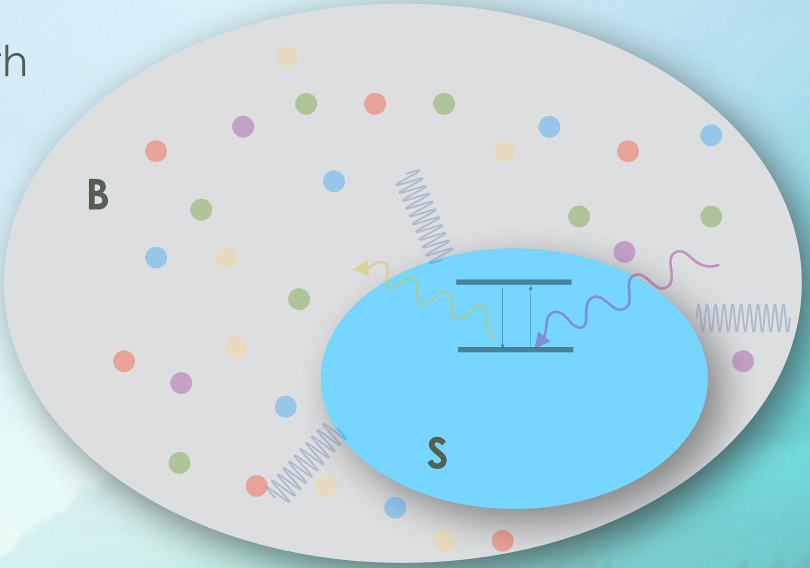
$$\Delta^2 H = \mathrm{Tr}[H^2]/d_S - \mathrm{Tr}[H]^2/d_S^2$$

—towards thermalization: atom in a thermal bath

$$H_S + H_B = (1/2)\omega_0\sigma_z + \sum_k \omega_k a_k^\dagger a_k$$

$$H_{\text{int}} = \lambda \sum_k f_k^* \sigma_+ \otimes a_k + f_k \sigma_- \otimes a_k^\dagger$$

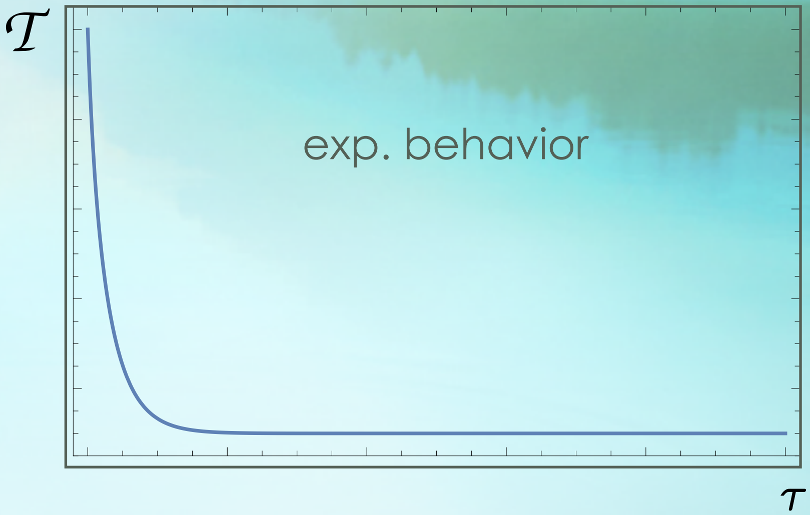
Jaynes-Cummings model



bosonic heat bath T

$$\lim_{\tau\to\infty} \varrho_S^{(\lambda)}(\tau) = \varrho_S^\beta$$

$$\lim_{\tau\to\infty} \mathcal{T}_S(\tau) = T$$



what is the connection of this equation with the usual known master equations, e.g., GKLS?

$$\dot{\varrho}_S(\tau) = -i[H'_S(\tau), \varrho_S(\tau)] - i\,\boxed{\mathrm{Tr}_B[H_{\mathrm{int}}, \chi(\tau)]}$$

?

K S G

In Ingarden's office, 1975

L

D. Chruściński and S. Pascazio, Open Sys. Inf. Dyn. **24**, 1740001 (2017)

$$\mathcal{L}_S \varrho_S(\tau) = -i[\widetilde{H}_S, \varrho_S(\tau)] + \boxed{\sum_m \gamma_m \left(2L_m \varrho_S L_m^\dagger - \{L_m^\dagger L_m, \varrho_S\}\right)}$$

limitations/assumptions of GKLS equation

derivation of GKLS starting from CPTP maps

—no initial correlation → $\varrho_S(\tau) = \mathcal{E}_S(\tau)[\varrho_S(0)] = \sum_n A_n(\tau)\varrho_S(0)A_n^\dagger(\tau)$

—time homogeneous dynamical semigroup property (divisibility of the dynamical map)

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

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)

→ $\boxed{\text{Markovian master equation}}$

beyond Born-Markov and RWA?

Projection operator techniques

Nakajima—Zwanzig projection operator technique

$$\frac{d}{dt}\mathcal{P}\tilde{\rho}(t) = \mathcal{P}\mathcal{V}(t)\mathcal{P}\tilde{\rho}(t) + \mathcal{P}\mathcal{V}(t)\mathcal{G}(t,0)\mathcal{Q}\tilde{\rho}(0) + \int_0^t du\mathcal{P}\mathcal{V}(t)\mathcal{G}(t,u)\mathcal{Q}\mathcal{V}(u)\mathcal{P}\tilde{\rho}(u)$$

$$\mathcal{P}\rho = \mathrm{Tr}_B(\rho)\otimes\rho_B \qquad \tilde{\rho}(t) = e^{i(H_A+H_B)t}\rho(t)e^{-i(H_A+H_B)t}$$

$$\mathcal{Q}\rho = (\mathbb{1}-\mathcal{P})\rho \qquad \mathcal{G}(t,s) = \mathcal{T}e^{\int_s^t dt'\mathcal{Q}\mathcal{V}(t')}$$

$$\mathcal{V}(t)\cdot \equiv -i[\tilde{V}(t),\cdot]$$

Path integral techniques

Monte Carlo techniques

etc…

Time-local master equation in the presence of memory effects (without semigroup property)?

Gorini-Kossakowski-Sudarshan theorem

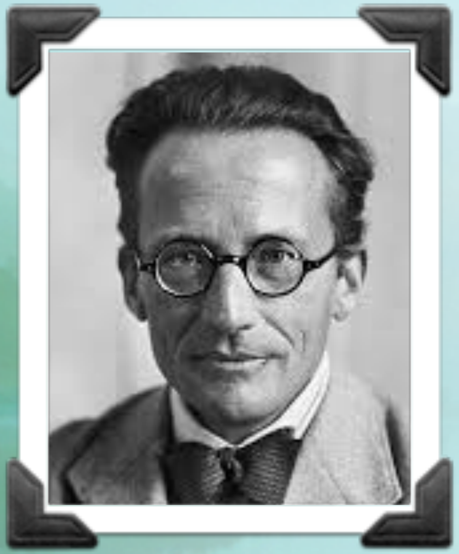
Any linear map with Hermiticity and trace preserving properties can be associated to a time-local generator as

$$\boxed{\mathcal{L}_S \varrho_S(\tau) = -i[\widetilde{H}_S, \varrho_S(\tau)] + \sum_m \gamma_m \left(2L_m \varrho_S L_m^\dagger - \{L_m^\dagger L_m, \varrho_S\}\right)}$$

— Theorem is just about existence (non-constructive)

— No clue on how to derive rates and jump operators

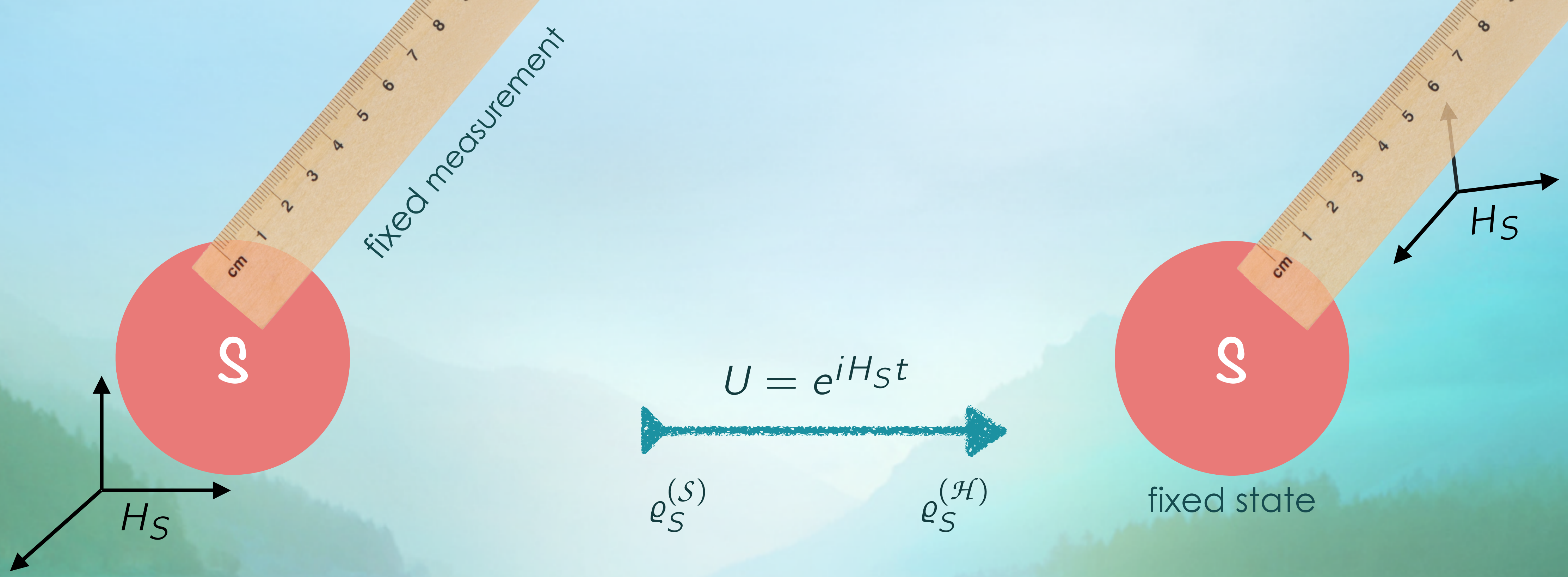
dynamical pictures in quantum mechanics



Schrödinger picture

Heisenberg picture

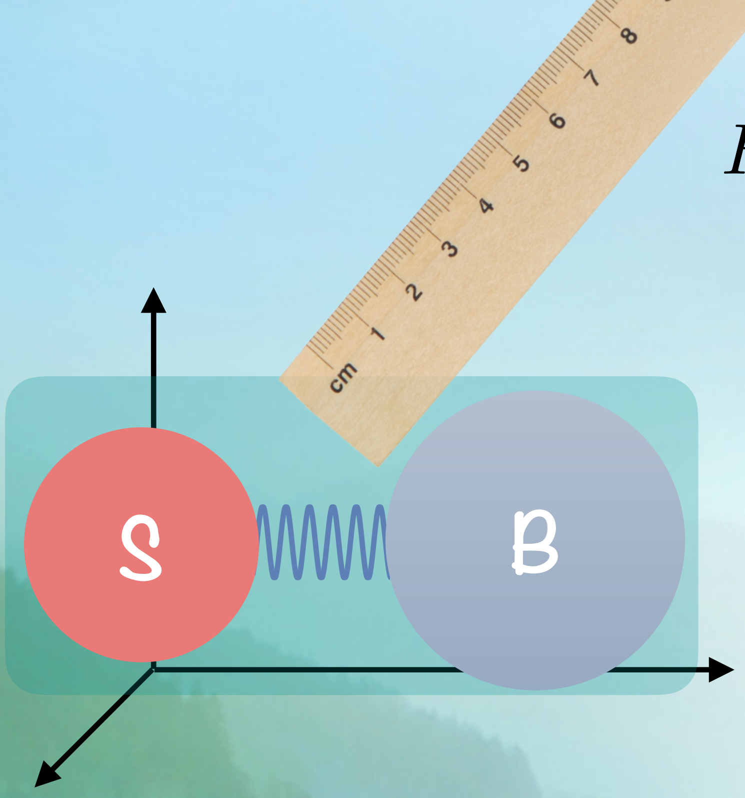
Dirac picture



Schrödinger picture:
ϱ_S coordinates evolve

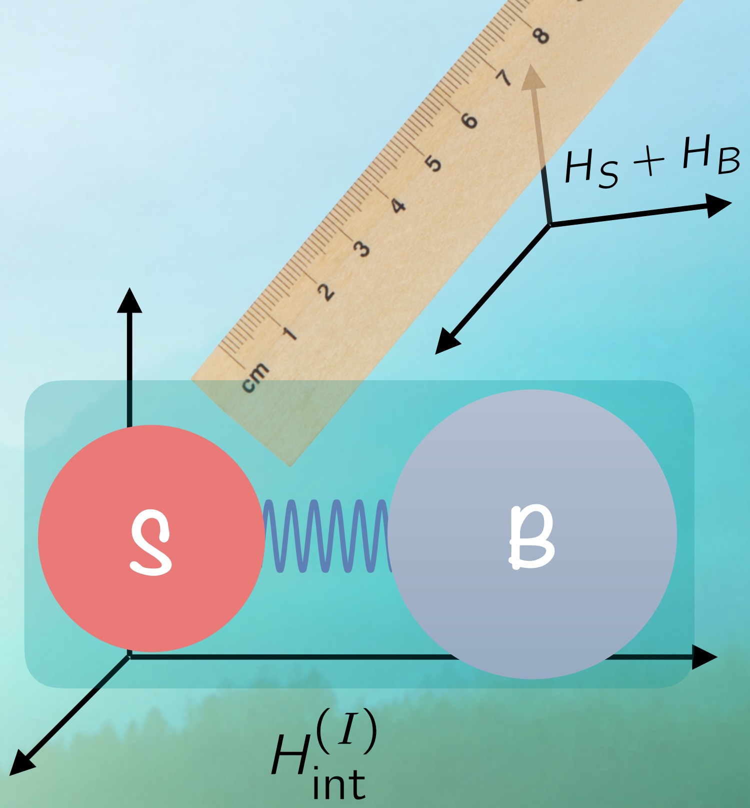
Heisenberg picture:
measurement direction evolves

$$H_{\mathrm{SB}} = H_{\mathrm{S}} + H_{\mathrm{B}} + \boxed{H_{\mathrm{I}}}$$



$$U = e^{i(H_S + H_B)t}$$

$$\varrho_{SB}^{(S)} \longrightarrow \varrho_{SB}^{(I)}$$



Schrödinger picture:
ϱ_{SB} coordinates evolve

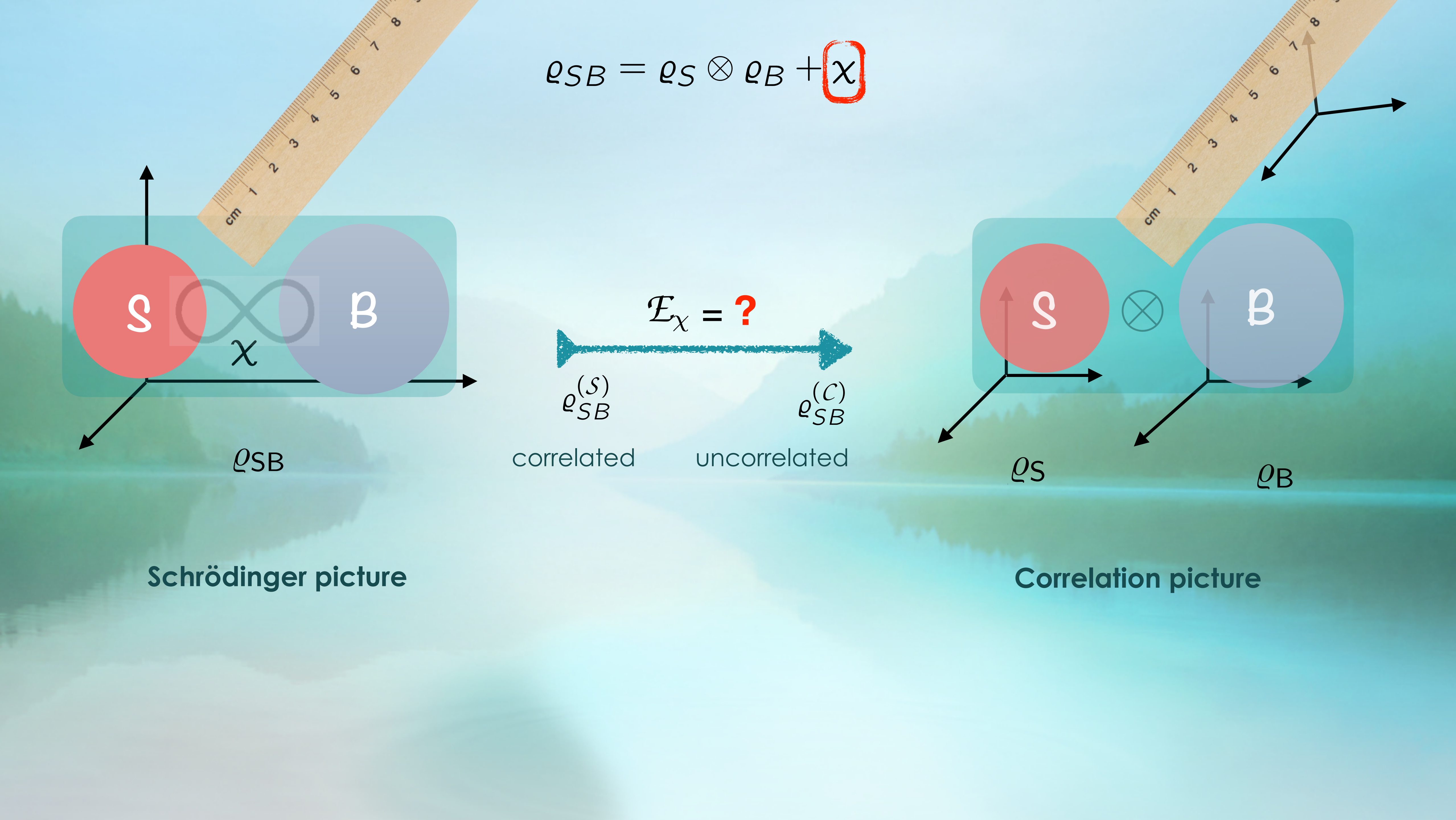
Dirac (interaction) picture:
state coordinates & measurements evolve

$$\varrho_{SB} = \varrho_S \otimes \varrho_B + \chi$$

a new dynamical picture?

correlation picture

[SA, A. T. Rezakhani, A. P. Babu, K. Mølmer, M. Möttönen, T. Ala-Nissila, arXiv: 1903.03861]


$\varrho_{SB} = \varrho_S \otimes \varrho_B + \boxed{\chi}$
S
B
χ
ϱ_{SB}
$\mathcal{E}_\chi$ = ?
$\varrho_{SB}^{(S)}$
$\varrho_{SB}^{(C)}$
correlated
uncorrelated
S
$\otimes$
B
ϱ_S
ϱ_B
Schrödinger picture
Correlation picture

—correlating transformation: a **weakly**-correlated state

interaction H_χ

$\varrho_\mathrm{S} \quad \otimes \quad \varrho_\mathrm{B}$

small

$U_\chi = e^{-iH_\chi}$

entangling gate

χ

$\varrho_\mathrm{SB} = \varrho_\mathrm{S} \otimes \varrho_\mathrm{B} + \chi$

small

$$\boxed{\varrho_\mathrm{SB} = U_\chi \varrho_\mathrm{S} \otimes \varrho_\mathrm{B} U_\chi^\dagger = \varrho_\mathrm{S} \otimes \varrho_\mathrm{B} - i[H_\chi, \varrho_\mathrm{S} \otimes \varrho_\mathrm{B}]}$$

equivalent form for the unitary transformation

$$\chi = -i[H_\chi, \varrho_\mathrm{S} \otimes \varrho_\mathrm{B}]$$

—correlating transformation: **general** case

?

$$\chi = -i[\![H_\chi, \varrho_{\mathrm{S}} \otimes \varrho_{\mathrm{B}}]\!]$$

non-Hermitian

where $[\![A, B]\!] = AB - B^\dagger A^\dagger$

$$\boxed{\varrho_{\mathrm{SB}} = \mathcal{E}_\chi[\varrho_{\mathrm{S}} \otimes \varrho_{\mathrm{B}}] := \varrho_{\mathrm{S}} \otimes \varrho_{\mathrm{B}} - i[\![H_\chi, \varrho_{\mathrm{S}} \otimes \varrho_{\mathrm{B}}]\!]}$$

Good news:

D. S. Djordjević, J. Comput. Appl. Math. **200**, 701 (2007)

Theorem 2.2. *Let $A \in \mathscr{L}(H,K)$ have a closed range and $B \in \mathscr{L}(H)$. Then the following statements are equivalent:*

(a) *There exists a solution $X \in \mathscr{L}(H,K)$ of Eq.* $\boxed{A^*X + X^*A = B}$

(b) $B = B^*$ *and* $(I - \boxed{A^\dagger}A)B(I - A^\dagger A) = 0$.

pseudo inverse

If (a) *or* (b) *is satisfied, then any solution of Eq.* (1) *has the form*

$$X = \tfrac{1}{2}(A^*)^\dagger B A^\dagger A + (A^*)^\dagger B(I - A^\dagger A) + (I - AA^\dagger)Y + AA^\dagger Z A,$$

where $Z \in \mathscr{L}(K)$ satisfies $A^*(Z + Z^*)A = 0$, and $Y \in \mathscr{L}(H,K)$ is arbitrary.

$$\chi(\tau) = -i\,[\![H_\chi(\tau), \varrho_S(\tau)\otimes\varrho_B(\tau)]\!] \quad \equiv \quad (\varrho_S(\tau)\otimes\varrho_B(\tau))(iH_\chi^\dagger(\tau)) + (iH_\chi^\dagger(\tau))^\dagger(\varrho_S(\tau)\otimes\varrho_B(\tau)) = \chi(\tau)$$

$$P_0(\tau)\chi(\tau)P_0(\tau) = 0$$

projector onto the null-space of $\varrho_S(\tau)\otimes\varrho_B(\tau)$

Derivation of the universal Lindblad-Like equation (ULL)

$$\dot{\varrho}_{\mathsf{SB}}(\tau) = -i[H_{\mathsf{SB}}, \varrho_{\mathsf{SB}}]$$

$$\mathcal{E}_{\chi}[\varrho_{\mathsf{S}} \otimes \varrho_{\mathsf{B}}] := \varrho_{\mathsf{S}} \otimes \varrho_{\mathsf{B}} - i[\![H_{\chi}, \varrho_{\mathsf{S}} \otimes \varrho_{\mathsf{B}}]\!]$$

$$\boxed{\dot{\varrho}_{\mathsf{SB}}(\tau) = -i[H_{\mathsf{SB}}, \varrho_{\mathsf{S}} \otimes \varrho_{\mathsf{B}}] - \big[H_{\mathsf{SB}}, [\![H_{\chi}, \varrho_{\mathsf{S}} \otimes \varrho_{\mathsf{B}}]\!]\big]}$$

$$H_{\mathsf{SB}} = H_{\mathsf{S}} + H_{\mathsf{B}} + H_{\mathrm{I}}$$

$\{\mathcal{S}_i\}$ operator basis of the system

$$H_{\mathrm{I}} = \sum \mathcal{S}_i \otimes \mathcal{B}_i$$

$$H_{\chi}(\tau) = \sum \mathcal{S}_i \otimes \mathcal{B}_i^{\chi}(\tau)$$

Inserting the decompositions and tracing out over the bath:

$$\dot{\varrho}_{\mathsf{S}} = -i\big[H_{\mathsf{S}} + \mathrm{Tr}_{\mathsf{B}}[H_{\mathrm{int}}\,\varrho_{\mathsf{B}}], \varrho_{\mathsf{S}}\big] - \sum_{i\neq 0,j}\big[\mathcal{S}_i, c_{ij}\mathcal{S}_j\varrho_{\mathsf{S}} - c^*_{ij}\varrho_{\mathsf{S}}\mathcal{S}_j\big]$$

environment correlation functions

$$\boxed{c_{ij}(\tau) = \mathrm{Tr}[\varrho_B(\tau)\mathcal{B}_i\mathcal{B}_j^{\chi}(\tau)]}$$

defining the Hermitian matrices:

$$\boldsymbol{b}(\tau) := \big(\boldsymbol{c}(\tau) - \boldsymbol{c}^{\dagger}(\tau)\big)/2i$$

$$\boldsymbol{a}(\tau) := \big(\boldsymbol{c}(\tau) + \boldsymbol{c}^{\dagger}(\tau)\big)/2$$

$$\boxed{\dot{\varrho}_{\mathsf{S}}(\tau) = -i\big[H_{\mathsf{S}} + \mathbb{h}_{\mathsf{L}}^{\chi}(\tau), \varrho_{\mathsf{S}}(\tau)\big] + \textstyle\sum_{i\neq 0, j\neq 0} a_{ij}(\tau)\big(2\mathcal{S}_j\,\varrho_{\mathsf{S}}(\tau)\mathcal{S}_i - \{\mathcal{S}_i\mathcal{S}_j, \varrho_{\mathsf{S}}(\tau)\}\big)}$$

Lamb-shift-like Hamiltonian: $\mathbb{h}_{\mathsf{L}}^{\chi}(\tau) = \langle H_{\mathrm{I}}\rangle_{\mathsf{B}} + 2\sum_{i\neq 0}\mathrm{Im}(c_{i0})\mathcal{S}_i + \sum_{i\neq 0, j\neq 0} b_{ij}(\tau)\mathcal{S}_i\mathcal{S}_j$

putting into standard form: diagonalization $U\boldsymbol{a}U^{\dagger} = \boldsymbol{\Gamma}$

defining $L_m^{\chi} = \sum_i U_{mi}S_i$

$$\boxed{\dot{\varrho}_{\mathsf{S}} = \mathcal{L}^{\chi}[\varrho_{\mathsf{S}}] = -\,i[H_{\mathsf{S}} + \mathbb{h}_{\mathsf{L}}^{\chi}, \varrho_{\mathsf{S}}] + \sum \gamma_m^{\chi}\big(2L_m^{\chi}\varrho_{\mathsf{S}}L_m^{\chi\dagger} - \{L_m^{\chi\dagger}L_m^{\chi}, \varrho_{\mathsf{S}}\}\big)}$$

valid in general (non-zero initial correlation, no need to weak-coupling (Born)/Markov/RWA assumption

Comparison:

$$\dot{\varrho}_S(\tau) = -i[H'_S(\tau), \varrho_S(\tau)] - \boxed{i\mathrm{Tr}_B[H_{\mathrm{I}}, \chi(\tau)]}$$

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

correlation dependent

How to get a Markovian reduction?

Expanding $\chi(\tau)$ around a zero-correlation point up to the **first order** (no need to Born-Markov and RWA)

$$\chi(\tau_0+\tau) = -i\tau\left[\widetilde{H}_{\mathrm{I}}(\tau_0+\tau), \varrho_{\mathsf{S}}(\tau_0+\tau)\otimes\varrho_{\mathsf{B}}(\tau_0+\tau)\right] + O(\tau^2)$$

$$\boxed{H_\chi \equiv \tau\,\widetilde{H}_{\mathrm{I}}(s) = \tau\sum\nolimits_{i\neq 0}\mathcal{S}_i\otimes\underbrace{(\mathcal{B}_i - \langle\mathcal{B}_i\rangle_{\mathsf{B}})}_{\mathcal{B}_i^\chi} - \underbrace{\sum\nolimits_{i\neq 0}\langle\mathcal{S}_i\rangle_{\mathsf{S}}\mathcal{B}_i}_{\mathcal{B}_0^\chi}}$$

$c_{ij} \propto \mathrm{Cov}(\mathcal{B}_i,\mathcal{B}_j)$ $\rightarrow$ $\boldsymbol{a}$ positive; $\boldsymbol{b}=0$

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}\tau}\varrho_S(\tau) = -i\left[H_S^{'}, \varrho_S(\tau)\right] + \sum_{ij}\underbrace{a_{ij}(\tau)}_{\gamma_m\geqslant 0}\Big(2\mathcal{S}_j\varrho_S\mathcal{S}_i - \{\mathcal{S}_i\mathcal{S}_j, \varrho_S\}\Big)}$$

$$H_{\mathsf{S}}^{'} = H_{\mathsf{S}} + \mathrm{Tr}_{\mathsf{B}}[H_{\mathrm{I}}\,\varrho_{\mathsf{B}}(\tau)]$$

Summary

- defined the Hamiltonian of the subsystems by looking at the dynamics of open quantum systems through two different approaches:

- in the first approach correlation considered as an independent entity to which a well-defined energy is associated (we completely separated correlations in description of subsystems)

- In the second approach, Lindblad form of the dynamics considered as the reference frame, where the operator in its coherent part considered as the subsystem Hamiltonian

- Lindblad form is a canonical form for general open-system dynamics

- Correlation plays an important role (as important as interaction) in both the coherent and the dissipative part of the dynamics

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